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Procedures for Including Secondary Electron Emission in Numerical Simulations of Plasma-Insulator Interactions

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Contents

Summary

When an energetic electron is incident on a solid surface, a considerable number of secondary electrons may be produced; this phenomenon is called *secondary electron emission.* The yield for most metals is less than one, but may be as large as 8 or more for insulators. Hence SEE is an important feature of plasma-solid surface interactions, and may have considerable effects on the behavior of components such as solar cells in low earth orbit. The purpose of this report is to provide a convenient scheme for including realistic SEE behavior in numerical simulations of plasma-suurface interactions.

Previous Monte Carlo simulations provide a data base for properties of secondary electron emission (SEE) from insulators and metals. Incident primary electrons are considered at energies up to 1200 eV. The behavior of secondary electrons is characterized by (1) yield *vs.* primary energy E_p, (2) distribution *vs.* secondary energy E_s and (3) distribution *vs.* angle of emission θ.

For primary energies above 50 eV the SEE yield curve can be conveniently parameterized by a Haffner formula. Special attention is paid in this report to the low energy range E_p up to 50 eV, where the number and energy of secondary electrons is limited by the finite band gap of the insulator. There is also a considerable probability for elastic backscattering or reflection of the primary electron in this energy range, and separate yield curves are given for reflected primary electrons.

The energy distribution of secondary electrons is described by an empirical formula with average energy about 8.0 eV. (A Maxwell-Boltzmann distribuftion, however, does not provide a good fit.) The angular distribution of secondaries is slightly *more* peaked in the forward direction than the customary $\cos\theta$ distribution.

The results of the MC simulations--yield and distribution curves--are conveniently represented by means of empirical formulas and appropriate parameters. Procedures and algorithms are described for using these results to find the SEE yield, and then to choose the energy and angle of emergence of each secondary electron. These procedures can readily be incorporated into numerical simulations of plasma-solid surface interactions in low earth orbit.

I. Introduction to Secondary Electron Emission

A. Description of SEE Processes and Behavior

When electrically charged particles with sufficient kinetic energy are incident on the surface of a solid material, the material emits electrons. This paper will only consider electrons as the incident charged particle. In keeping with the current literature these incident electrons will be called "primary electrons," and the electrons from the material that are excited by the primary electron will be called "secondary electrons." The secondary electron yield δ is the ratio of external secondary electron current to primary electron current. The yield may also be regarded as the average number of external secondary electrons per primary electron.

Different types of materials exhibit characteristically different yields. The basic source of the difference in yield between the types of materials is the electron energy band structure. A diagram showing the energy bands for a metal and for an insulator is shown below.

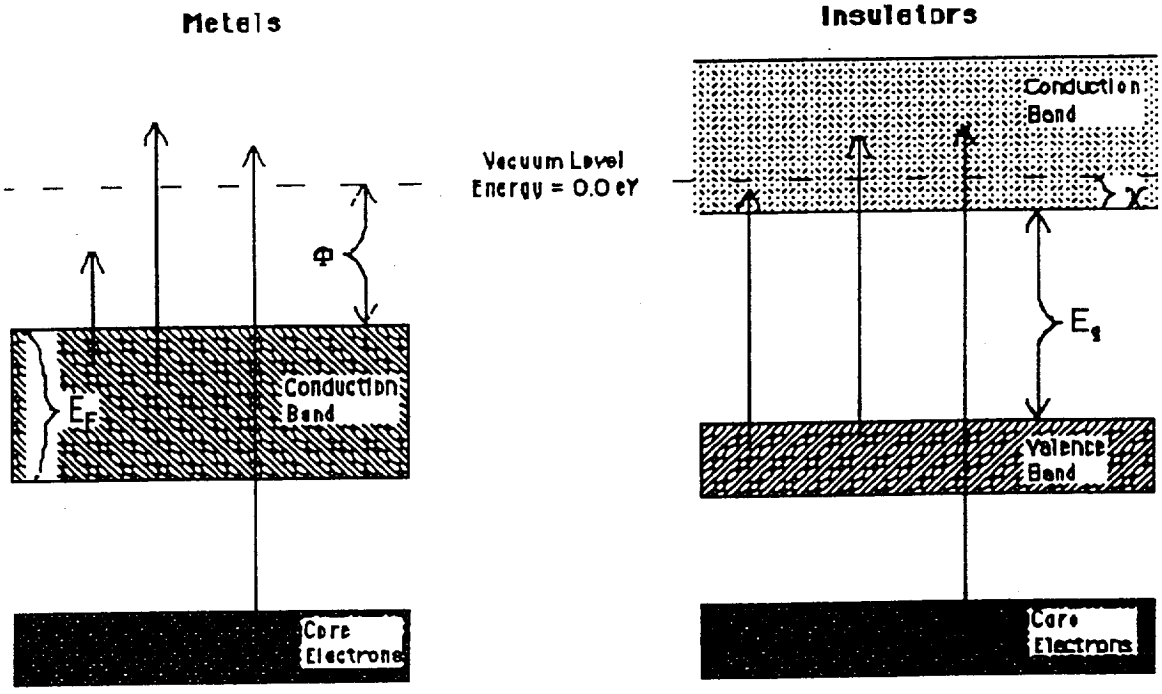


Fig. 1 Energy level diagrams for metals and for insulators.

The single headed arrows represent the amount of energy an internal electron may acquire by interacting with the primary electron or other internal secondary electrons. As indicated in the diagram, if the internal secondary electron has sufficient energy to climb to the vacuum level, it may be able to leave the material and become an external secondary electron. It is important to keep in mind, though, that the internal secondary electron must also be traveling toward the surface of the material if it is to become an external secondary. On its way to the surface, an internal secondary may interact with many other internal electrons. With each interaction the secondary electron will lose energy and/or suffer a change in direction. It is the number of these interactions and the distance to the vacuum level that ultimately determines whether or not an electron will become an external secondary electron.

In metals the work function Φ is the energy that all electrons must be able to overcome to become external secondary electrons. Just below the work function is the top of the conduction band E_F. The conduction band is partially filled, with occupied levels just below E_F and unoccupied levels immediately above E_F. The core represents those energy levels that are already completely filled. These are the only energy levels in which an electron can exist. Therefore, if a primary electron penetrates the surface of a metal with sufficient kinetic energy, it will be in the conduction band since it is not able to enter the core by the Pauli exclusion principle.

Since the conduction band is partially filled, both the primary electron and the internal secondary electrons will often suffer inelastic collisions in which only a small amount of energy (a few eV) is lost to conduction band electrons. These frequent small-energy-loss collisions cannot lead to external secondary electrons since the energy transferred between the colliding electrons is less than Φ. Therefore much of the initially available energy is "wasted" and the yield is small.

The situation is quite different for insulators. Insulators have an electron affinity χ that all electrons must overcome to become secondary electrons. χ is the energy difference between the surface of the material and the bottom of the empty conduction band. Below the conduction band is the valence band, which is completely filled for good insulators. The core levels are at still lower energies. Between the bottom of the conduction band and the top of the valence band is the band gap E_g; no electrons are allowed in this energy region. In insulators the width of the band gap is the major determinant of the secondary electron yield.

As illustrated schematically by the diagram on page 4, a good insulator is characterized by a large band gap. In this case most excitation processes raise an internal electron above the vacuum level, allowing for possible secondary electron emission. This is the basic reason why the maximum yield for insulators is much larger than for metals. Semi-conductors have a small band gap. For such materials the situation is similar to that of metals; hence the maximum yield for semiconductors is between those for metals and insulators. For very large band gap insulators the maximum yield tends to decrease somewhat, perhaps because the primary electron can penetrate to greater depths before exciting the internal electrons.

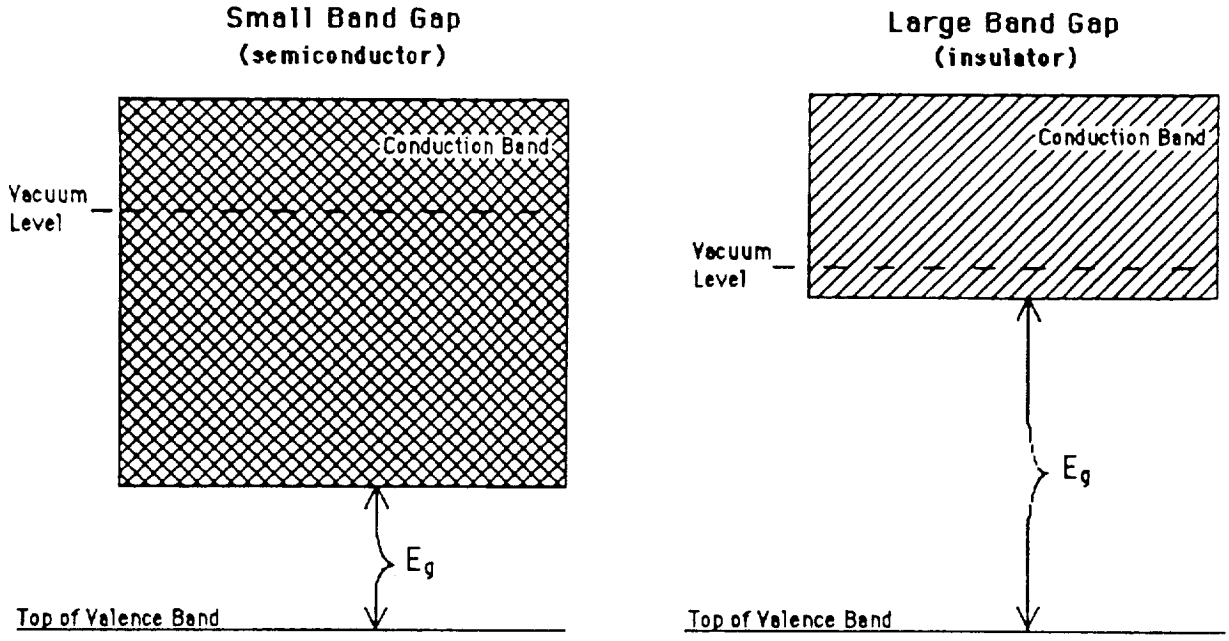


Fig. 2 Energy level diagrams for a semiconductor and for a large band gap insulator.

The diagram below shows the maximum yield versus the band gap for several real solids (open circles), and the results of G. A. Rezvani's Monte Carlo simulations (solid circles). The materials are identified in the table on the following page.

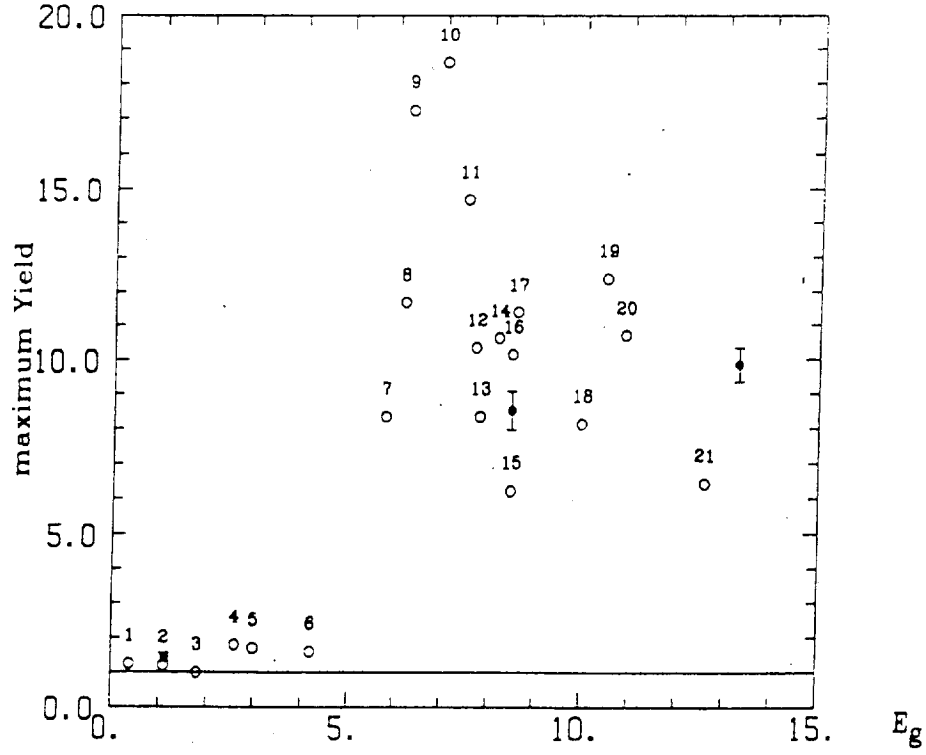


Fig. 3 Maximum SEE yield *versus* band gap E_g(eV) for a number of solids.

No.	material	E_g (eV)	χ (eV)	σ_m	E_m (eV)
1	PbS	0.4	4.7	1.25	500
2	Sb_2Te_3	1.1	4.34	1.2	700
3	GeS	1.8	4.0	1.0	400
4	PbO	2.6	3.6	1.8	600
5	TeO_2	3.0	3.4	1.7	600
6	Sb_2O_3	4.2	2.8	1.6	500
7	NaI	5.8	1.5	8.35	1390
8	KI	6.2	1.1	11.68	1430
9	CsI	6.3	0.1	17.23	2150
10	$CsBr$	7.0	0.2	18.61	2340
11	$CsCl$	7.5	0.3	14.68	1470
12	$NaBr$	7.7	-	10.34	1430
13	KBr	7.8	0.9	8.35	630
14	$RbCl$	8.2	0.51	10.62	1310
15	$LiBr$	8.5	1.0	6.22	580
16	KCl	8.5	0.6	10.14	1000
17	$NaCl$	8.6	0.65	11.39	1300
18	$LiCl$	10.0	0.54	8.14	1000
19	NaF	10.5	-	12.38	1290
20	KF	10.9	0.1	10.7	1100
21	LiF	12.6	1.0	6.42	540

Table 1 Band gap, electron affinity, maximum yield, and energy of primary electron at maximum yield for several insulators.

The torturous nature of the SEE process is illustrated by the diagram on page 6 from one of Rezvani's simulations. The solid line shows the path, projected onto the yz- plane, of a 400 eV primary electron incident normally on solid argon. The dotted lines show the paths of the internal secondary and tertiary electrons. (A tertiary electron is one excited by a higher energy internal secondary electron, *etc.*) According to Rezvani, the primary electron suffered 200 interactions (the maximum allowed by his simulation) and generated 22 internal secondary electrons and 7 tertiary electrons. In this simulation run 12 of the internal secondary electrons reached the surface and managed to escape.

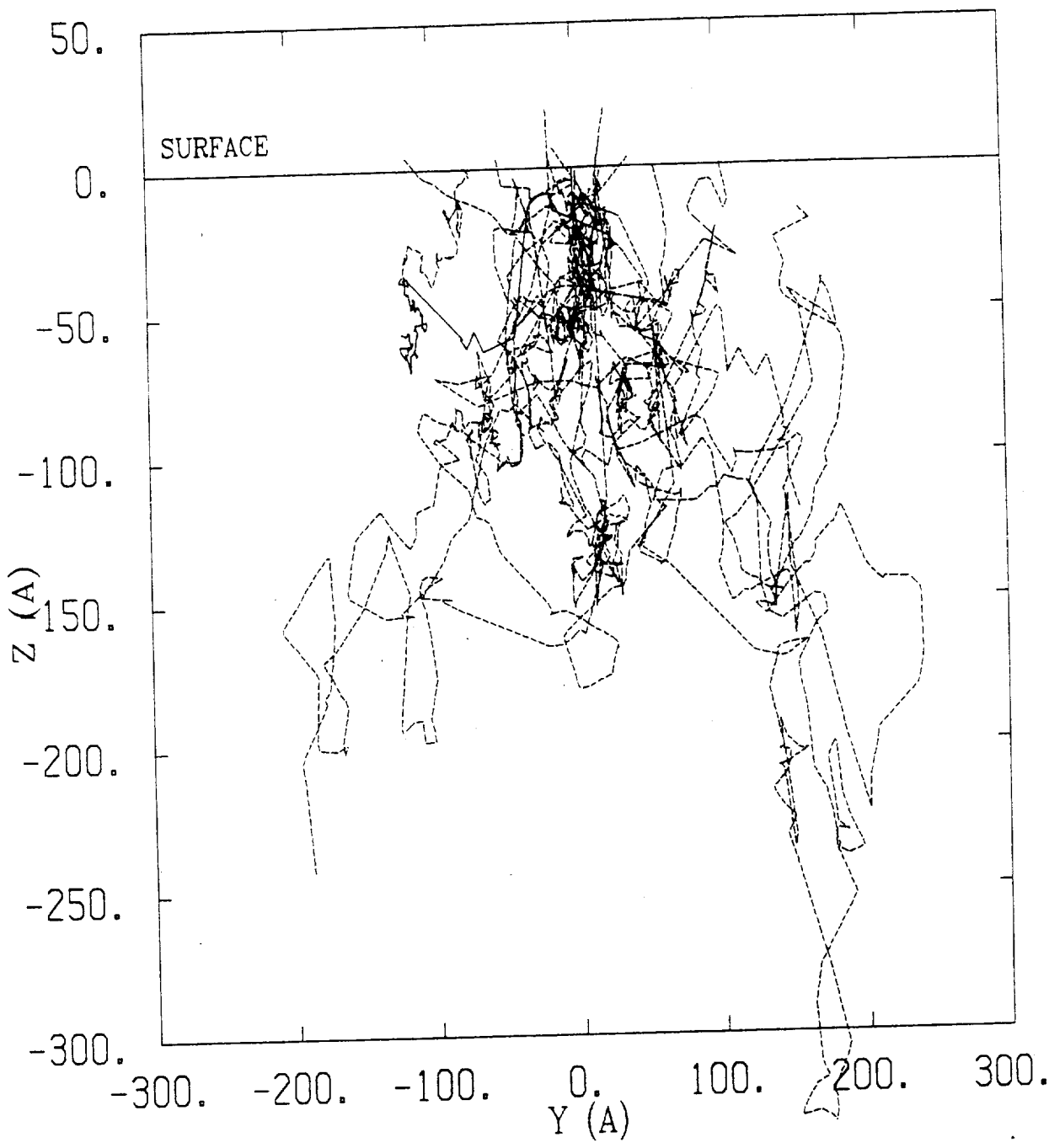


Fig. 4 Family tree of 400 eV primary electron in argon. The figure shows the projection of the trajectory onto the yz-plane. The trajectory of the primary electron is shown with a solid line, and the trajectories of the secondaries with broken lines.

B. Characterization of External Secondary Electrons

The most important characteristics of secondary electron emission are the secondary electron yield *versus* the primary electron energy, the energy distribution of the external secondary electrons, and the angular distribution of the secondaries.

Most of the research has focused on the first characteristic, secondary electron yield as a function of primary energy. It has been shown that for all bulk solids the secondary electron yield will start from zero at $E_p = 0$ eV, rise rapidly to a maximum yield δ_m at E_m, then slowly decrease with $E_p > E_m$. If the secondary electron yield for some material were plotted versus energy of the primary energy, the result would be a variation of the "universal" yield curve. Such a curve is shown below.

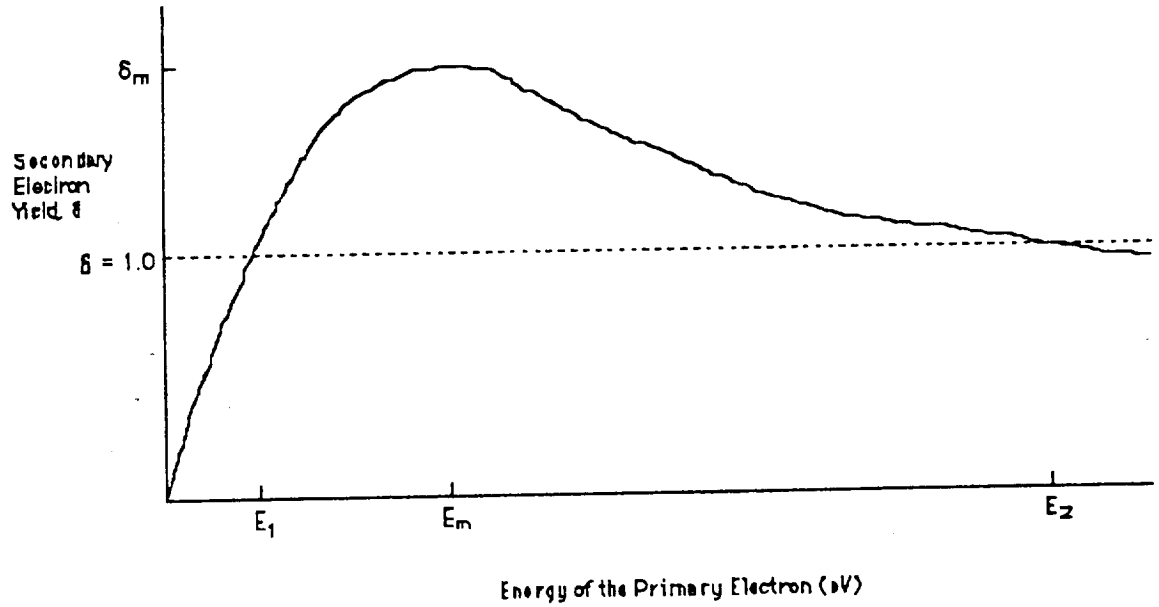


Fig. 5 Universal SEE yield curve.

Typical values of the maximum yield for various materials are shown in the following table. Notice that the yield is greater than one, often by a large amount, for semiconductors and insulators.

Material	Maximum Yield
Metals	less than 1
Semiconductors	1 - 2
Polymers	2 - 3
Insulators	6 - 12

It is convenient to define E_1 and E_2 as the energies of the primary electron for which the yield is 1.0. These energies are significant for plasma-insulator interactions; for $E_1 < E_p < E_2$ the yield will be greater than 1.0, and the insulator will charge positively. Likewise, for $E_p < E_1$ and $E_p > E_2$ the yield will be less than 1.0 and the material will charge negatively. For insulators E_1 is about 16 eV, E_m is around 200 - 400 eV, and E_2 is typically greater than 1000 eV.

The next important characteristic of secondary electron emission is the energy distribution of the secondaries. The major features of this distribution are illustrated on the next page for a typical primary energy E_p = 150 eV. The maximum S at 10 eV is nearly independent of E_p, and is therefore representative of "true" secondaries. These are electrons that were initially present as bound electrons in the solid, were excited by the primary electron, and finally managed to escape from the surface to become external secondary electrons.

The maximum B is located at the primary energy E_p, and can only be from primary electrons that have undergone elastic back-scattering. The shape of the small maximum U is characteristic of the material and originates from inelastically scattered primaries, i.e. primary electrons that suffer only one or two inelastic collisions before being scattered back out of the solid. The region between 50 eV and the maximum U originates from a mixture of true secondaries and inelastically scattered primaries. The two types of secondary electrons in this region are not distinguishable by means of external measurements.

The results of secondary electron emission described in Part II of this report are based on Monte Carlo simulations of the SEE processes. To simulate the elastic scattering, a general overall form of the elastic scattering cross section typical of low atomic mass elements (12 to 40 amu) was used. Since detailed features of elastic scattering for specific elements were not included, the simulations were not able to reproduce the back-scattering peaks at U and B for primary energies $E_p > 50$ eV. However, for primary energies $0 < E_p < 50$ eV the back-scattering peak at B was obtained. In all cases the simulations give good results for the main secondary peak at S, which is more important for the purpose of modeling the plasma-insulator interactions.

The final important characteristic of secondary electron emission is the angular distribution of the external secondaries. Because of the large number of collisions suffered by the primary and secondary electrons inside the solid (tens or hundreds in typical cases), the angular distribution of excited electrons near the surface should be essentially isotropic. But since the excited electron must be traveling toward the surface to be emitted, the angular distribution of external secondaries should approximate a cosine weighted distribution, *i.e.*, weighted in the direction of the outward normal to the surface. Rezvani found that this distribution is essentially independent of the energy of the primary electron and of the angle of incidence of the primary electron. A straight forward cosine distribution is generally accepted for experimental results. However, the Monte Carlo simulations give a distribution peaked slightly more in the forward direction, as will be presented in Part II.

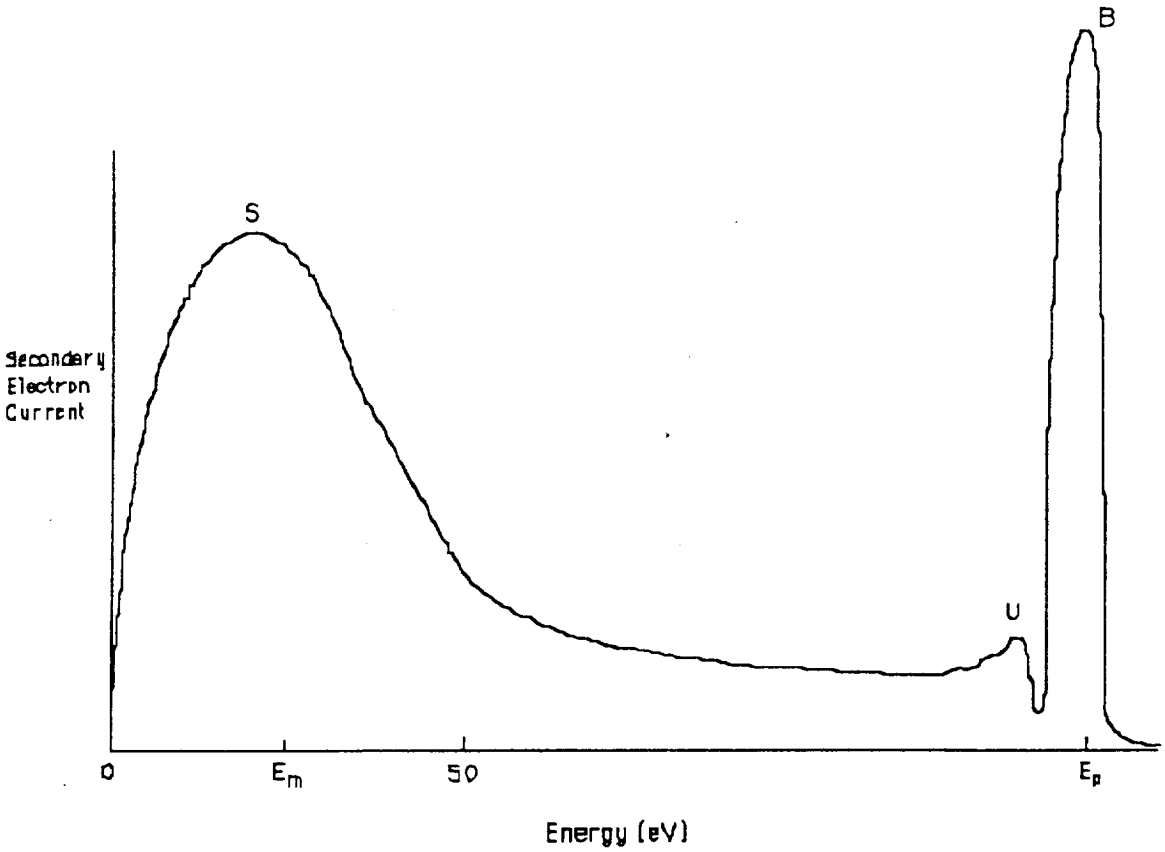


Fig. 6 Schematic energy distribution of secondary electrons. This diagram is not drawn to any particular scale and does not represent any particular material. However, the broad features of the diagram are true of almost all materials.

In these simulations, Rezvani observed that after a primary electron, or excited internal electron, suffered two or three interactions with other electrons it would "forget" about its initial direction of travel. Furthermore, most internal secondaries are excited with modest energies of 5 to 50 eV, and after excitation become "ignorant" of the energy of the primary electron. This behavior appears vividly in the jagged nature of the tracks for both primaries and secondaries (Fig. 4). Consequently, both the energy distribution and the angular distribution of secondary electrons are nearly independent of the primary energy and of the angle of incidence of the primary.

This independent behavior on the part of the secondary electrons is observed in all bulk solid materials. For very thin films, however, more detailed features of the paths would have to be taken into consideration. From Fig. 4 the mean penetration depth of the primaries is about 50 Å, and most secondaries do not wander to depths below 200 Å. Therefore, "thin" means only a few hundred Ångstrom units. We shall concern ourselves with bulk materials in the solid state, and refer the interested reader to the literature for thin films.

In the next part of this paper we will develop a method of simulating secondary electron emission for use in numerical simulations of plasma-insulator interactions.

II. Method of Including SEE in Numerical Simulations of Plasma-Insulator Interactions

When an insulating solid is situated in a plasma environment, the resulting interactions affect the properties of both the insulator and the plasma. The insulator will acquire a surface charge, which may be negative or positive depending on the potential of the insulator and the properties of the plasma. In addition the density and velocity of the particles in the plasma will be affected out to a distance of several Debye lengths away from the insulating surface. One way of studying the behavior and physics of these interactions is to create a computer simulation to follow the motion of the charged particles in the volume of the plasma near the surface. In any such program an important feature of the plasma-insulator interactions is the production of secondary electrons when an electron from the plasma impacts the surface of the insulator. The purpose of this report is to describe a method for incorporating the SEE response of an insulator (or metal) surface into a computer simulation of the plasma-insulator interactions.

The situation we wish to describe goes as follows. An electron in the plasma, moving under the influence of the electric fields produced by all the charges in the system, impacts at a certain time somewhere on the surface of the insulator. From the velocity components of this primary electron, we can determine its kinetic energy and angle of incidence onto the surface. At this point in the simulation, we need to determine how many secondary electrons are emitted. If there are some, we will need to determine the kinetic energy and direction of motion of each of the secondaries. In the following sections of this part we describe the distributions and procedures that can be used for this purpose.

A. Total Yield vs. Primary Electron Energy

The secondary electron yield δ depends on the kinetic energy and angle of incidence of the primary electron, and is also influenced considerably by the properties of the material that forms the surface. Typical behavior for model quartz and aluminum is shown on the figures on page 14. At zero primary energy the yield is zero. (But even for primary energies of a few eV there are a considerable number of elastically reflected primaries; see section D.) As the primary energy increases, the yield increases rapidly, simply because more energy is available for producing secondaries. The yield reaches a maximum at some energy E_m, and then decreases slowly for higher primary energies. This is because higher energy primaries penetrate more deeply into the material, which implies that the excited electrons have further to travel before escaping from the surface.

A convenient fitting formula for δ_o, the yield at normal incidence ($\theta = 0$), is provided by the Haffner formula.

$$\delta_o(E_p) = C\left(e^{-aE_p} - e^{-bE_p}\right) \tag{2.1}$$

The parameters a, b, and C are empirically fitted to experimental or simulation data for a particular material. To relate δ_m and E_m to these parameters, we start by setting the derivative of δ equal to 0:

$$0 = \frac{\partial \delta_o(E_p)}{\partial E_p} = C\left(-ae^{-aE_p} + be^{-bE_p}\right) \tag{2.2}$$

$$\Rightarrow \quad ae^{-aE_p} = be^{-bE_p} \tag{2.3}$$

$$\Rightarrow \quad E_m = \frac{\log(b/a)}{(b - a)} \text{ (keV)} \tag{2.4}$$

This is the energy of the primary electron for which the yield δ is a maximum. Assuming the maximum yield δ_m is known from the data, the parameter C can be found by inserting E_m into the Haffner formula:

$$\delta_m = C\left(e^{-aE_m} - e^{-bE_m}\right) \tag{2.5}$$

$$\Rightarrow \quad C = \frac{\delta_m}{\left(e^{-aE_m} - e^{-bE_m}\right)} \tag{2.6}$$

For the plasma-insulator simulations we should like to use quartz as a prototype for a good insulator. But the complexity of the composition and crystal structure of quartz prevent us from a direct simulation of the secondary electron emission, and the

experimental data are old and questionable. Therefore to find parameters for quartz we look at our simulation results for KCl, which has a band gap of 8.5 eV that is comparable to 8.0 eV for quartz. Similarly, the electron affinity for quartz is 1.0 eV, whereas the electron affinity of KCl is 0.6 eV. We have performed extensive simulations with model KCl for $\chi = 0.0$ eV and $\chi = 2.0$ eV. Since the electron affinity for quartz is halfway between these values, we propose a simple linear interpolation between the results for the two models of KCl, as illustrated below.

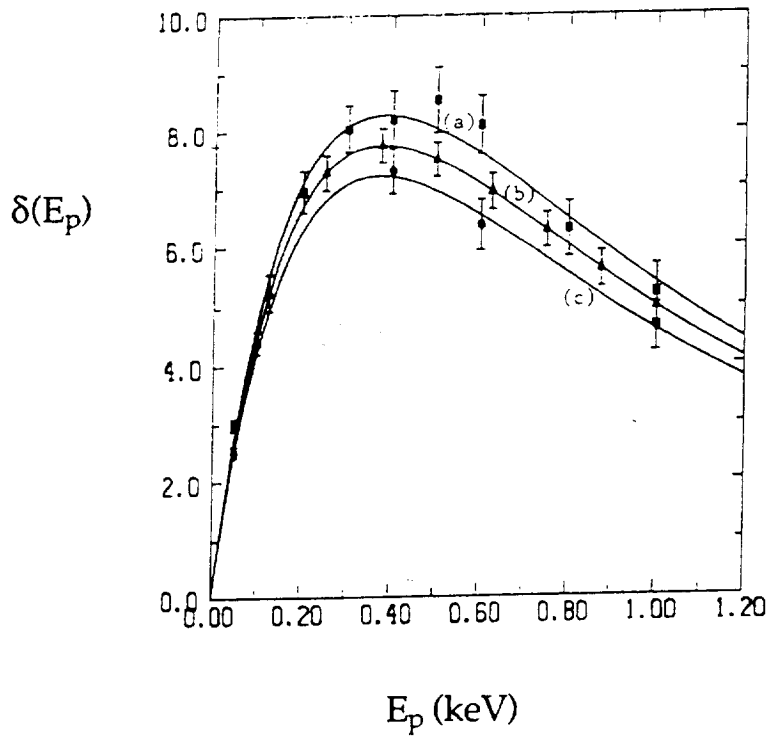


Fig. 7 Haffner yield curves for several model solids.

(a) Model KCL with $\chi = 0.0$ eV
(b) Model quartz with $\chi = 1.0$ eV
(c) Model KCL with $\chi = 2.0$ eV

The secondary electron yield also increases with increasing angle of incidence of the primary electron, where θ is measured from the normal to the surface. As θ increases, the depth to which the primary electron penetrates decreases; thus the excited internal electrons have less distance to travel to the surface, and the secondary yield becomes larger. An empirical formula to represent this effect is:

$$\delta(\theta) = \delta_o \, e^{c(1-\cos\theta)} \qquad (2.7)$$

Some references suggest a value of c = 2 for polymers, but this choice would make $\delta(90^\circ)/\delta_o = e^2 = 7.4$. From a few Monte Carlo simulations of SEE at fairly large angles ($\theta = 60^\circ$ to 80°), our experience indicates that this factor is too large. We prefer to use c = 1, which gives $\delta(90^\circ)/\delta_o = e = 2.7$ instead.

On page 14 are plots of the Haffner formula for quartz and aluminum with angle θ varying from 90° for the greatest yield down to 0° in increments of 30°. The values of the parameters we used are shown below:

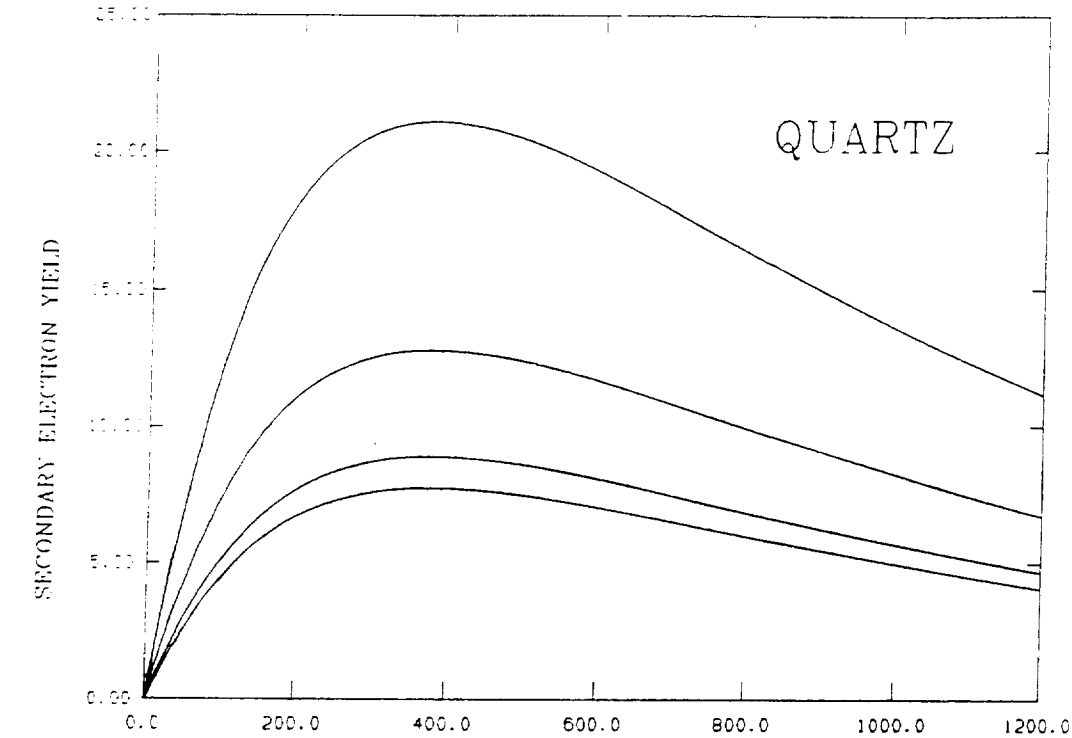
Material	**Parameter**	E_m
Quartz	a = 1.02/keV b = 5.47/keV C = 14.02	377 eV
Aluminum	a = 0.5/keV b = 8.3/keV C = 1.23	360 eV

The data for aluminum are taken from "Experimental Result B" in Rezvani's Ph.D. thesis, volume 1, page 211. The curves for quartz are fitted to the results of Rezvani's Monte Carlo simulations, as shown in Fig. 7.

In a numerical simulation that would involve secondary electron emission, one would typically keep track of the positions and velocities of the particles in the simulation volume. When a primary electron strikes the insulator surface, the required variables for the Haffner formula are calculated as follows.

$$E_p = \frac{m_e \sqrt{V_x^2 + V_y^2 + V_z^2}}{2 \times 1.602189 \times 10^{-19}} \text{ eV} \qquad (2.8)$$

$$\theta_p = \arctan\left(\frac{\sqrt{V_x^2 + V_y^2}}{V_z}\right) \text{ radians} \qquad (2.9)$$



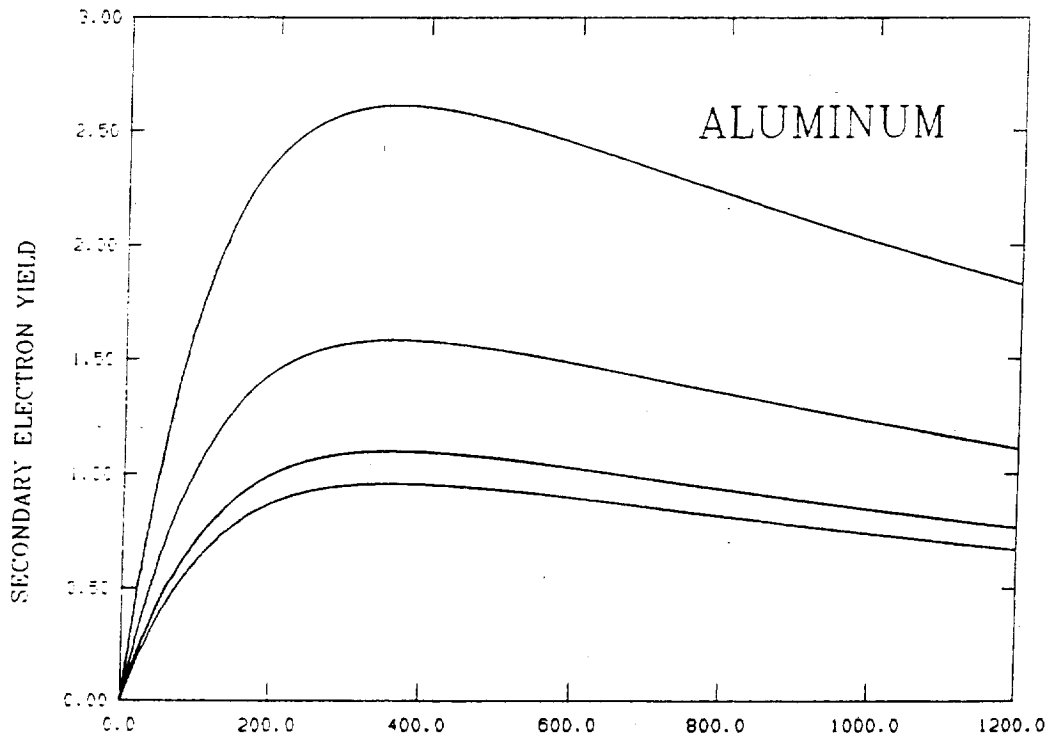


Fig. 8 Haffner yield curves for various angles of incidence of the primary electron.

The yield δ from the Haffner formula will be a fractional number. This number is a ratio of primary electron current to secondary electron current. However, in a numerical simulation it may be necessary to obtain an integer value for the yield N(δ). A simple solution to this requirement can be found if, as in many simulations, a large number of primary particles are involved. In this case the number δ can be considered to be the average number of secondary electrons emitted from the material per incident primary electron.

The method we use to accomplish this result begins with a call to a subroutine YIELDMAX, which calculates the Haffner formula as in equation (2.7) and returns the value YIELD. We then add a random fraction to the yield and truncate the sum to an integer:

$$y = \text{RAN(seed)}$$
$$N_{pos} = \text{INT(yield + y)}$$

Y is a random fraction from 0.0 inclusive to 1.0 exclusive, and N_{pos} is the integer value corresponding to the yield δ. (N_{pos} is an abbreviation for Number possible, signifying that this is the greatest possible number of secondaries that can be liberated by the current primary. But because of energy considerations the final yield may be less than N_{pos}. More on this later in section C.)

To understand this algorithm consider the following example. Let's assume that δ = 1.7, so some of the time the integer yield will be 1 and some of the time the integer yield will be 2. Since the fraction that is added to the result of the Haffner formula is chosen at random, 70% of the time the sum will be equal to or greater than 2 and 30% of the time it will be less than 2. Repeating the process for a large number of secondaries, an average value of 1.7 will be obtained for the yield.

B. Energy Distribution of Secondary Electrons

Each secondary electron that is produced in a numerical simulation needs to be assigned an energy and a direction. At present our concentration will be on assigning an energy to each secondary electron with a suitable distribution function.

We developed our distribution function based on Rezvani's simulation data for 100 primary electrons with E_p = 50.0 eV at normal incidence on solid argon. The histogram of these results is shown in the figure on page 18. Since the relative number of secondaries climbs rapidly at low secondary electron energies and falls off rapidly as E_s increases past 5.0 eV, we decided to try a distribution function of the form:

$$f(E_s) = A\sqrt{E_s}\, e^{-(E_s/E_o)^2} \tag{2.10}$$

$$\Rightarrow \quad dP(E_s) = f(E_s)\, dE_s \tag{2.11}$$

Now we can establish some properties of this distribution function. First we normalize the integrated probability to unity.

$$1 = P(E_s) = \int_0^\infty dP(E_s) = \int_0^\infty f(E_s)\, dE_s \tag{2.12}$$

$$= A \int_0^\infty \sqrt{E_s}\; e^{-(E_s/E_o)^2}\, dE_s \tag{2.13}$$

Making the substitution $u = (E_s/E_o)^2$ produces an integral that can be expressed in terms of the gamma function $\Gamma(u)$.

$$1 = \frac{A\, E_o^{3/2}}{2} \int_0^\infty u^{3/4\,-\,1}\, e^{-u}\, du \tag{2.14}$$

$$= \frac{1}{2} A\, E_o^{3/2}\, \Gamma(0.75) \tag{2.15}$$

$$\Rightarrow \quad A = 1.632\, E_o^{-3/2} \tag{2.16}$$

To find the maximum of the distribution function, we set the derivative with respect to E_s equal to zero:

$$0 = \frac{\partial f(E_s)}{\partial E_s} \quad \Rightarrow \quad \frac{E_s^{3/2}}{E_o^2} = \frac{1}{4} E_s^{-1/2} \tag{2.17}$$

$$\Rightarrow \quad E_{S_{max}} = \frac{E_o}{2} \tag{2.18}$$

The average energy is found from

$$E_{av} = \int_0^\infty E_s \, f(E_s) \, dE_s = A \int_0^\infty E_s^{3/2} \, e^{-(E_s/E_o)^2} \, dE_s \tag{2.19}$$

With the usual substitution $u = (E_s/E_o)^2$ the result is

$$E_{av} = \frac{\Gamma(1.75)}{\Gamma(0.75)} E_o = \frac{0.9064}{1.2255} E_o = 0.7396 \, E_o \tag{2.20}$$

A least squares fit of this distribution to Rezvani's data gives $E_o = 10.28$ eV. Rezvani's data and the fitted distribution function are shown on the next page.

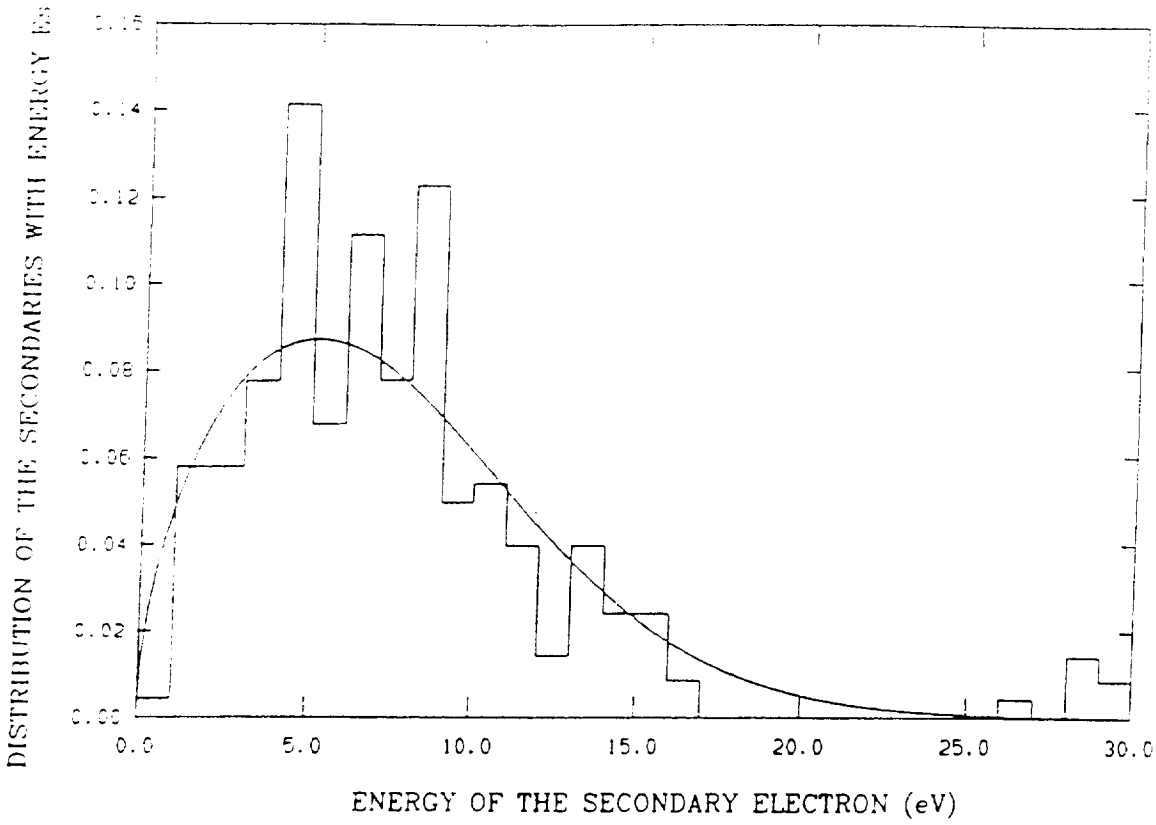


Fig. 9 Energy distribution of secondary electrons. The histogram gives the results of the Monte Carlo simulations for E_p = 50 eV in argon. The curve shows the best fit of the empirical formula of equation (2.10).

Notice that this distribution is <u>not</u> a Maxwell-Boltzman energy distribution. In fact, early attempts to fit the histogram with a MB distribution gave poor results. If the peak of the MB distribution is chosen at about 5 eV to fit the histogram, then the high energy end of the MB distribution is much too large for the results of the distribution as displayed on the histogram. Physically, there is no reason to expect the secondary electrons to fit a MB distribution, which corresponds to thermal equilibrium. Although the secondary electrons make a number of collisions with atoms in the solid before escaping (the number of collisions can be anywhere between one and several hundred), they do not by any means come into thermal equilibrium with the solid or with each other. Consider, for example, the average energy of the secondary electrons at 7.5 eV; this is much greater than kT_{room} = 0.025 eV.

It will be seen that most of the secondary electrons have modest energies, in the range 5 to 15 eV. This is significant for the plasma-insulator simulations in two ways. First, the secondary electrons have enough energy to wander away from the surface for a significant distance (several centimeters) which allows them to drift in the electric field present near the surface. But when these secondary electrons fall back onto the surface, they produce a yield less than one, as given by the Haffner formula eq. (2.1). However, as will be discussed in section D of this part, at the lower energies there is a significant probability that the impacting electron will be elastically reflected. These effects can produce a significant current sheath just above the surface of the insulator, which can be considered to be a surface current. Without secondary electron emission this effective surface current would not be present.

Once the distribution function $f(E_s)$ is known, there are two more steps in order to select energies in accordance with the distribution function. First, we need to obtain the integrated probability from 0 up to each E_s.

$$P(E_s) = \int_0^{E_s} f(E_s') \, dE_s' \tag{2.21}$$

The values of $P(E_s)$ increase monotonically from zero at $E_s = 0$ up to unity at $E_s = \infty$. Actually, we cut off the distribution at $E_s = 30$ eV because the values of $f(E_s)$ are negligible for $E_s \geq 30$ eV. Second, we need to select a random number $0 \leq r < 1$. With this number we find the value of E_s for which

$$P(E_s) = r \tag{2.22}$$

The solution of this equation can be written symbolically in terms of an inverse functional relationship.

$$E_s = P^{-1}(r) \tag{2.23}$$

Sometimes it is possible to carry out both steps of this process analytically, and then the last equation can be written as a specific algorithm to give E_s directly from r. This state of affairs occurs, for instance, for a two dimensional MB distribution (but not for one or three dimensions!). In our case the integrated probability would involve an incomplete gamma function; we have yet to come across the inverse of such a function. Our alternative is to integrate the distribution function numerically and make a table of $P(E_s)$ vs. E_s. Then to economically accomplish the solution of equation (2.22), we use interpolation to construct the inverse table, namely E_s vs. $P(E_s)$, at uniform intervals of $P(E_s)$. We can then quickly solve equation (2.23) by table look-up and interpolation. Furthermore, since both tables have as their first column evenly spaced entries, we can use a one line algorithm to find the entries we want without searching through the tables. For example, say we have a value for $P(E_s)$ and want to find the

corresponding E_s. Assuming there are 100 evenly spaced entries for $P(E_s)$, which ranges from 0 to 1, we find the index I as

$$I = INT(100*r) + 1 \tag{2.24}$$

Then the desired value of E_s lies between $E_s(I)$ and $E_s(I+1)$, and we can quickly find E_s by linear interpolation.

The procedure we have developed in this section is based on the assumption that the energy distribution for E_s of the secondary electrons is independent of the energy E_p of the primary electron. For $E_s \geq 50$ eV this assumption is reasonably valid. Once an internal secondary electron is excited, it has no further knowledge of E_p, and most internal excitations occur in the range from 0 to 40 eV. We have also checked this assumption with the results of the Monte Carlo simulations of SEE for argon with $E_p = 50$ eV and $E_p = 400$ eV; there is no discernible difference between the two histograms for the secondary electron energy distribution (although there is a sizable difference in yield for the two cases). When $E_p < 50$ eV, however, less energy is available for formation of secondary electrons, and additional considerations must be take into account. These considerations will be considered in the next section. There is also a much larger chance for reflection of the primary electron, as discussed in section D.

C. Considerations on Yield and Energy of Secondary Electrons at Low Primary Electron Energies

We can now look in detail at the energy considerations involved as secondaries are liberated from bulk solid material. Consider the energy level diagram below. When a primary electron strikes an insulator with some energy E_p, it may drop at most to the bottom of the empty conduction band since all of the states in the valence band

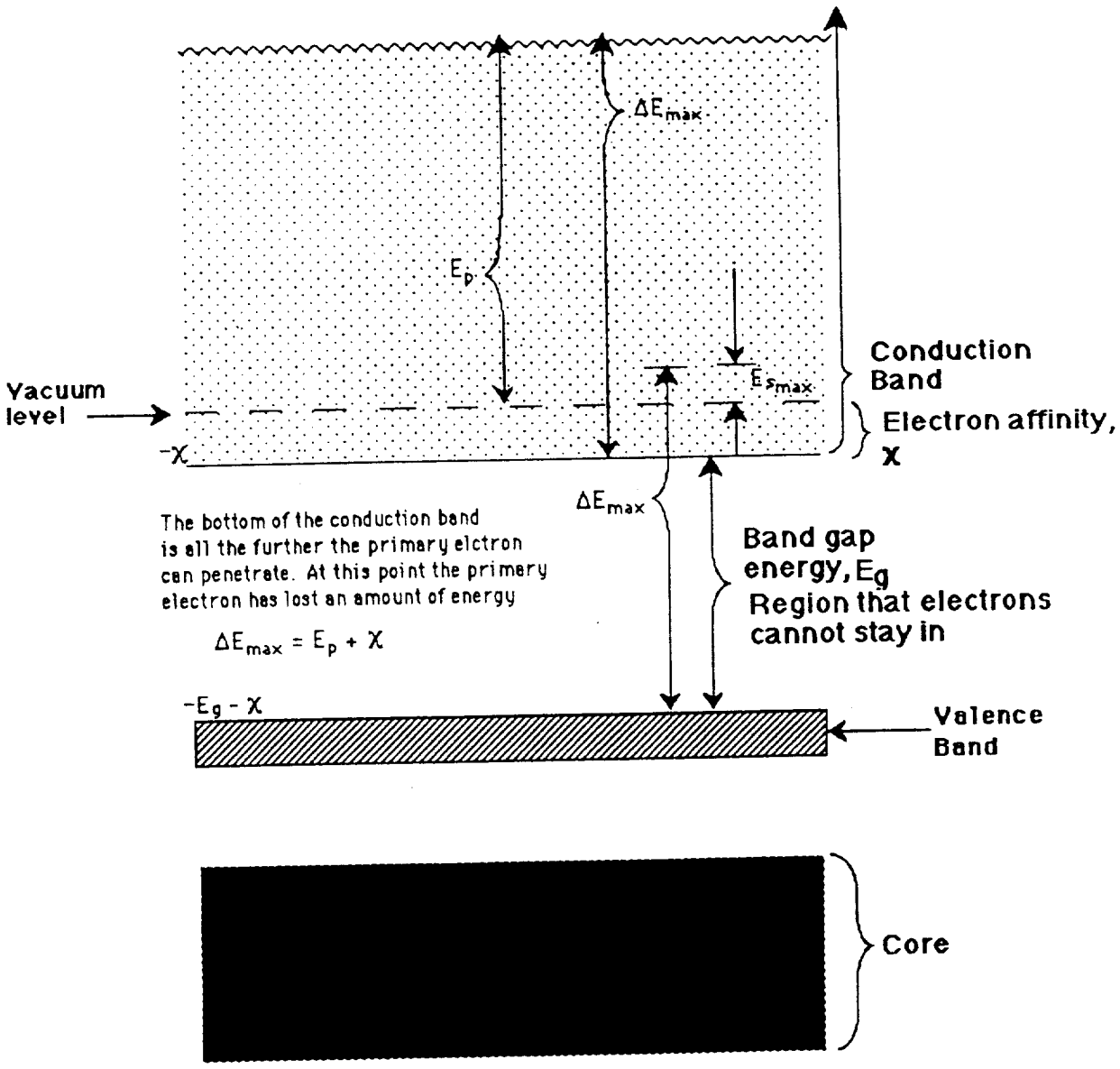


Fig. 10 Energy level diagram for an insulator.

are filled. The most energy that can be delivered to the material by the primary electron, then, is the sum of its kinetic energy and the electron affinity χ:

$$\Delta E_{max} = E_p + \chi \tag{2.25}$$

Any internal electron that becomes sufficiently excited because of the energy liberated by the primary electron may become a secondary electron. Each secondary electron will come from either the valence band or the core. However, the deeper the excited internal electron is, the more energy it will require to get to the surface of the material and become a secondary electron. The most loosely bound electrons in the solid are at the top of the valence band. These will require a minimum energy:

$$E_b = E_g + \chi \tag{2.26}$$

just to reach the vacuum level. E_b is the surface barrier. Any excited internal electron having less energy than this will have no chance of becoming an external secondary electron.

On the other hand, if an excited internal electron is able to make it to the surface to become a secondary electron, the greatest energy it can possibly have is:

$$\begin{aligned} E_{S_{max}} &= \Delta E_{max} - E_b \\ &= (E_p + \chi) - (E_g + \chi) \\ E_{S_{max}} &= E_p - E_g \end{aligned} \tag{2.27}$$

Now it is necessary to insist that $Es_{max} \geq 0$ in order to have any production of secondary electrons. Hence there is a minimum value of E_p, which is obtained by setting $Es_{max} = 0$.

$$E_o = E_{p_{min}} = E_g \tag{2.28}$$

If a primary electron strikes the surface with $E_p < E_o$, then the yield of secondary electrons must be zero. There is still the possibility, however, that the primary electron can be elastically scattered back out of the solid. The treatment of reflected electrons will be discussed in section D.

We can now consider the procedure for assigning an energy to the first secondary electron when $E_p > E_o$. We calculate $\delta(E_p)$ from the Haffner formula, equation (2.7), and then obtain the integer value N_{pos} by the algorithm on page 15. The maximum energy available for the secondary electron is given by equation (2.27).

$$E_{s_{max\,1}} = E_p - E_g$$

Therefore we must truncate the energy distribution function of section B at $Es_{max\,1}$. The total probability that the secondary electron will have an energy between 0 and $Es_{max\,1}$ is 1.00. In order to obtain this result, we must renormalize the distribution function between 0 and $Es_{max\,1}$ as follows. We have a table of integrated probability for the complete distribution function according to

$$P(E_s) = \int_0^{E_s} p(x)\,dx \qquad (2.29)$$

By table look-up from this table we obtain

$$P_{max} = P(E_{s_{max\,1}}) \qquad (2.30)$$

Then we define the truncated distribution by

$$p'(E_s) = \frac{p(E_s)}{P_{max}}$$

and the same relation follows for the integrated probability.

$$P'(E_s) = \frac{P(E_s)}{P_{max}} \qquad (2.31)$$

It will be seen that the integrated probability up to and including $Es_{max\,1}$ is unity, as it should be.

In order to select an energy E_{s1} for the first secondary electron, we choose a random number r such that $0 \le r \le 1$. We want to set r equal to the integrated probability for some E_s.

$$r = P'(E_s) = \frac{P(E_s)}{P_{max}} \tag{2.32}$$

So we want to find E_s such that

$$P(E_s) = r\,P_{max} \tag{2.33}$$

We can find the desired value of E_s by table look-up and interpolation in the inverse table for $E_s(P)$, just as in the preceding section. The advantage of this approach is that we do not need to actually construct a new table of $P'(E_s)$ for each value of $Es_{max\,1}$. We simply look for a *different* value of $P(E_s)$, according to equation (2.33).

When $\delta(E_p,\theta)$ is large enough to give $N_{pos} \ge 2$, there is the possibility of producing a second (and perhaps a third, etc.) secondary electron. But there is only a finite amount of energy to produce secondaries and enable them to overcome the surface barrier. So we need some way of ensuring conservation of energy. We can do so with the following equations.

$$\begin{aligned} \Delta E_{max\,2} &= \Delta E_{max} - E_{s1} - E_b \\ &= E_p + \chi - E_{s1} - (E_g + \chi) \\ &= E_p - E_{s1} - E_g \end{aligned} \tag{2.34}$$

$$\begin{aligned} E_{s_{max\,2}} &= \Delta E_{max\,2} - \langle E_g + \chi \rangle \\ &= E_p - E_{s1} - 2E_g - \chi \end{aligned} \tag{2.35}$$

If $Es_{max\,2} \le 0$, we do not have enough energy to form another secondary electron, and we do not allow for reflection of the primary electron in this case, so we quit. But if $Es_{max\,2} > 0$, we proceed to select E_{s2} by the method of the preceding paragraph.

When $N_{pos} \geq 3$, we continue to look for the possibility of producing more secondaries. The above process continues until either the number of secondaries produced reaches N_{pos}, or $Es_{max\ i} < 0$. The actual number of secondary electrons produced is called N_{act}. Of course in all circumstances, $N_{act} \leq N_{pos}$.

We can use the same procedure when dealing with secondary electron emission from metals. However, metals do not have a band gap nor an electron affinity. It is the work function ϕ that comprises the surface barrier in metals. To correctly treat metals, replace χ in equation (2.25) and $E_g + \chi$ in equation (2.26) with ϕ. Then equation (2.27) becomes

$$E_{s_{max}} = \Delta E_{max} - E_b$$

$$= (E_p + \phi) - \phi = E_p \qquad (2.36)$$

Thus it is possible to form secondaries in metals for any $E_p > 0$; there is no threshold energy. The reason for this difference in behavior from insulators is due to the difference in band structures. In a metal there are unoccupied electron energy levels immediately above the Fermi level, so it is possible for the primary electron to drop right down to the Fermi level. In insulators, this behavior is not possible because of the finite band gap.

For most metals the maximum yield at normal incidence is less than one, but for glancing incidence it is possible for values of $N_{pos} = 2$ or 3 to occur (see bottom figure on page 14). Then from equation (2.35) we find

$$E_{s_{max2}} = E_p - E_{s1} - \phi \qquad (2.37)$$

and so on, and proceed in the same way as for insulators.

D. Reflection of Primary Electrons at Low Energies

When a primary electron enters an insulator, the most probable type of collision is elastic scattering. When $E_p < E_o$, the threshold energy, the *only* kind of scattering process that can occur is elastic scattering. Even when E_p is somewhat greater than E_0, inelastic scattering events have smaller probabilities and elastic scattering still tends to dominate. The Monte Carlo simulations for low E_p primaries often show a track in which the primary electron goes through anywhere from a few up to more

than a hundred collisions before eventually escaping from the surface. In these cases the energy of the escaping electron must still equal E_p, and we speak of elastic backscattering or reflected primary electrons.

Fig. 11 on the following page shows the backscattering yield, or number of elastically reflected primary electrons per total number of primary electrons, for E_p ranging from 0 to 50 eV. It will be seen from the figure that backscattering is quite important for low energy primaries from 0 to 15 eV. On the figure, the X's are the backscattering yield obtained from the Monte Carlo simulations for argon. To this data we have fitted the following empirical formula:

$$\delta_r(E_p < 16.8) = A\, E_p^{\,b}\, e^{-(E_p/c)^d}$$

$$\delta_r(E_p \geq 16.8) = 0.06 \qquad (2.38)$$

The values of the coefficients as determined by least squares fitting are:

A = 0.40	c = 8.1
b = 0.70	d = 2.0

This form gives a rapid rise from $E_p = 0$, a maximum less than one at $E_p \approx 5.0$ eV, a rapid decline toward $E_p = 16$ eV, and then a constant value for $E_p > 17$ eV. The figure shows the empirical curve of equation (2.38), and the O's show the result of a trial run with the average yield at each energy determined by using random numbers. The results are in good agreement with the general behavior of Rezvani's simulations.

Since a reflected primary has undergone a number of collisions inside the solid before escaping from the surface, it has lost track of its original angle of incidence. (See Fig. 4.) Thus this phenomenon differs markedly from specular reflection, in which the angle of reflection is equal to the angle of incidence. We have looked at the angular distribution of reflected primaries at several energies, and find that the results for reflected primaries are similar to those for "true" secondaries. Therefore we can use the same angular distribution described in the next section for reflected primaries as well as for true secondaries.

When the plasma-insulator simulation tells us that an electron strikes the surface of the insulator, we proceed as follows. First we calculate the reflection yield δ_{ref} from the empirical formula above, and then determine an integer yield in the usual manner.

$$N_{refl} = \text{INT}(\delta_{refl} + r) \qquad (2.39)$$

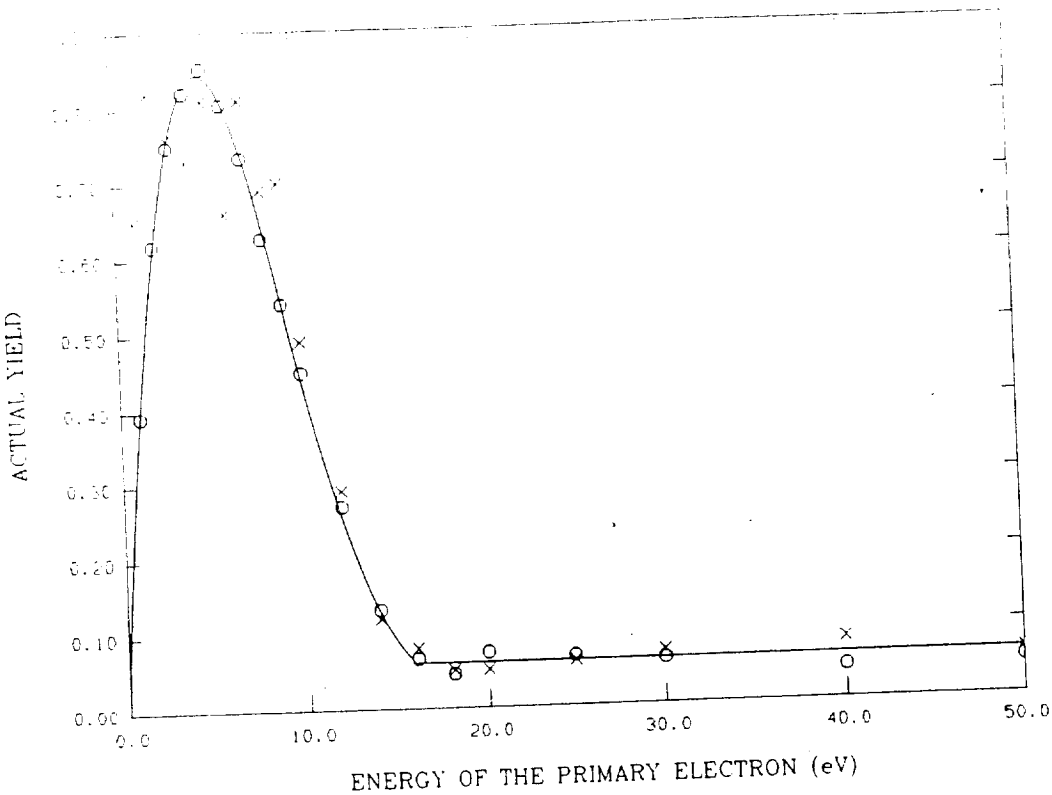


Fig. 11 Yield of elastically reflected primary electrons. The X's are obtained from the Monte-Carlo simulations, and the curve is from the fitted empirical formula. The O's show the result of a trial run with the average yield determined by random numbers.

where r is a random number with $0 \le r < 1$. The result for N_{ref} must be either zero or one. When $N_{ref} = 1$, we assign E_p as the energy of the reflected primary and choose θ according to the standard angular distribution. In this case there can be no yield of secondary electrons. When $N_{ref} = 0$, we next calculate the yield from the Haffner formula as given by equation (2.7) (when $E_p > E_o$), and proceed to handle secondary electrons as described previously.

The large yield of reflected primaries at low E_p is bound to reduce the secondary electron yield in this energy range. This effect appears in the figure at the end of the report showing true secondary yield vs. E_p. The effect is especially noticable from 8 to 15 eV. The reflected primaries also show up as a backscattering peak at E_p in the histograms for the energy distribution of secondary electrons, as well as on the figure showing total yield as a function of E_p. These figures are also located at the end of this report.

In the case of metals, primary electrons are not reflected to any significant extent. Even when E_p is as low as 2 or 3 eV, inelastic scattering processes are still possible in which an electron in the conduction band with an energy near the Fermi level is excited by a small amount of energy. The possibiity of these small energy inelastic excitations is the basic difference between the behavior of metals and insulators. Consequently we do not consider reflected primaries when simulating SEE for metals.

E. Angular Distribution of Secondary Electrons

The task of assigning directions in spherical-polar coordinates is somewhat simpler than assigning energies to the secondaries. By examining Rezvani's simulation results, we find that there exists azimuthal symmetry about the point of emission, as expected physically. Thus the azimuthal angle ϕ can be chosen randomly between 0 and 2π.

$$\phi = 2\pi \times \alpha \tag{2.40}$$

where α is a random number such that $0 \leq \alpha < 1$.

Next we need to select the polar angle θ, measured from the outward normal to the surface (see Fig. 13 on page 31). For this purpose we plot results from Rezvani's simulations on solid argon, as shown in Fig. 12 below. For these plots it is convenient to introduce a new variable $x = \cos\theta$. Each distribution is normalized properly by using the basic definition of a distribution function, namely,

$$\Delta N = N\, f(x)\, \Delta x \tag{2.41}$$

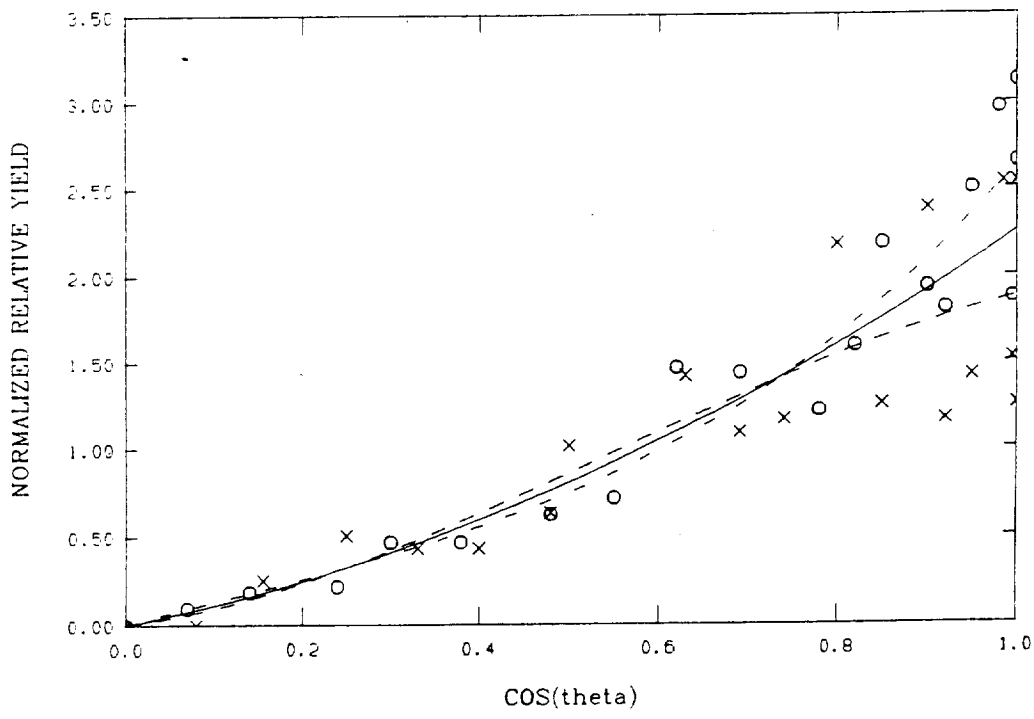


Fig. 12 Angular distribution of secondary electrons. The data points are simulation results for SEE from solid argon. Dot-dash line and O's are for E_p = 400 eV. Dash line and X's are for E_p = 50 eV. The solid line is the best fit to the combined sets of data.

where N is the trial number of events, and ΔN is the number of events in the range of width Δx. Then the normalized probability is given by

$$f(x) = \frac{1}{N}\frac{\Delta N}{\Delta x} \tag{2.42}$$

There is a moderate amount of scatter in the simulation results because simulations were run for only 100 primary electrons at each value of E_p. But within these limits there is no significant difference between the angular distributions for the two very different values of E_p at 50 eV and at 400 eV. Therefore we combine the results of both distributions for the purpose of fitting an angular distribution function. In order to accomodate some of the curvature, we perform a least squares fit with a function of the form:

$$f(\theta) = A\cos\theta + B\cos^2\theta + C\cos^3\theta \tag{2.43}$$

Since only those electrons that make an acute angle with the outward normal will be emitted (Fig. 13), we normalize the distribution for θ ranging from 0 to $\pi/2$:

$$1 = P(\tfrac{\pi}{2}) = \int_0^{\pi/2} dp(\theta) = N\int_0^{\pi/2} f(\theta)\sin(\theta)\,d\theta \tag{2.44}$$

$$= N\int_0^{\pi/2} \left\{A\cos(\theta) + B\cos^2(\theta) + C\cos^3(\theta)\right\}\sin(\theta)\,d\theta \tag{2.45}$$

With the substitution $x = \cos\theta$ we obtain the result

$$1 = N\int_0^1 \left\{Ax + Bx^2 + Cx^3\right\}dx = N\left\{\frac{A}{2} + \frac{B}{3} + \frac{C}{4}\right\} \tag{2.46}$$

$$\Rightarrow \quad N = \left\{\frac{A}{2} + \frac{B}{3} + \frac{C}{4}\right\}^{-1} \tag{2.47}$$

We determined the coefficients A, B, and C by fitting this distribution function to the combined sets of simulation data for 50 eV and for 400 eV primary electrons. The result is that A = 0.9900, B = 1.2375, and C = 0.0263. A plot of the best fit line is shown along with the data in Fig.12.

In most of the literature on SEE an angular distribution proportional to $\cos\theta$ is assumed. Then the normalized distribution function would be :

$$f(\theta) = 2\cos\theta \tag{2.48}$$

This is a simple form and is qualitatively justifiable on the basis of physical arguments. If we consider a cloud of internal secondaries, for instance, just beneath the surface, the situation is similar to a cloud of molecules in a gas near some surface. The velocity distribution of molecules actually striking the surface is weighted with a factor

$$v_n = v\cos\theta \tag{2.49}$$

where v_n is the normal component of velocity. A similar distribution should be reasonably appropriate for secondary electrons that manage to escape from the surface.

But the detailed processes of secondary electron emission are more complicated than this simple picture. The figure on page 6 of Part I shows the jagged and irregular paths followed by each secondary electron in the solid. Furthermore, the internal secondary electrons are not in thermal equilibrium with the solid or with each other, as mentioned previously. There is even a potential barrier to overcome at the surface, so it is even less likely for a secondary electron with a small v_n to escape. We believe that this is the reason that our angular distribution, as fitted to the Monte Carlo SEE results, is slightly more peaked in the forward direction than a simple $\cos\theta$ distribution.

We have examined angular distributions for additional Monte Carlo simulations of SEE with Rezvani's programs, especially for low primary energies of 10 to 50 eV. In all cases we find a good fit with the angular distribution function described here. Even for reflected primary electrons, which predominate for E_p below 10 eV, we find the reflected electrons follow a similar angular distribution. This result occurs because most of the reflected primaries make a number of elastic collisions (5 to 200) inside the solid before escaping from the surface. So we can use the same angular distribution function for all cases of reflected primaries and true secondaries.

Once the angular distribution function is specified, we can develop the procedure for assiging an angle θ to each secondary electron. First we tabulate the values of the integrated, normalized angular distribution function *versus* decreasing values of θ, as θ ranges from π/2 to 0.0; we consider cos θ to be the variable of integration. Then, as for assigning energies to the secondaries, we choose a random number between 0.0 inclusive and 1.0 exclusive to represent the value of the integrated distribution function at some angle θ. In order to facilitate the process of finding the angle θ that corresponds to this value of the integrated distribution function, we construct the inverse look-up table listing θ vs. integrated distribution, at equal intervals of integrated distribution. Then we can readily find the appropriate angle θ by table look-up and interpolation. To check the program design for this purpose, we have used random numbers in the process of selecting values of θ for 1000 secondary electrons, with the results shown at the end of this report.

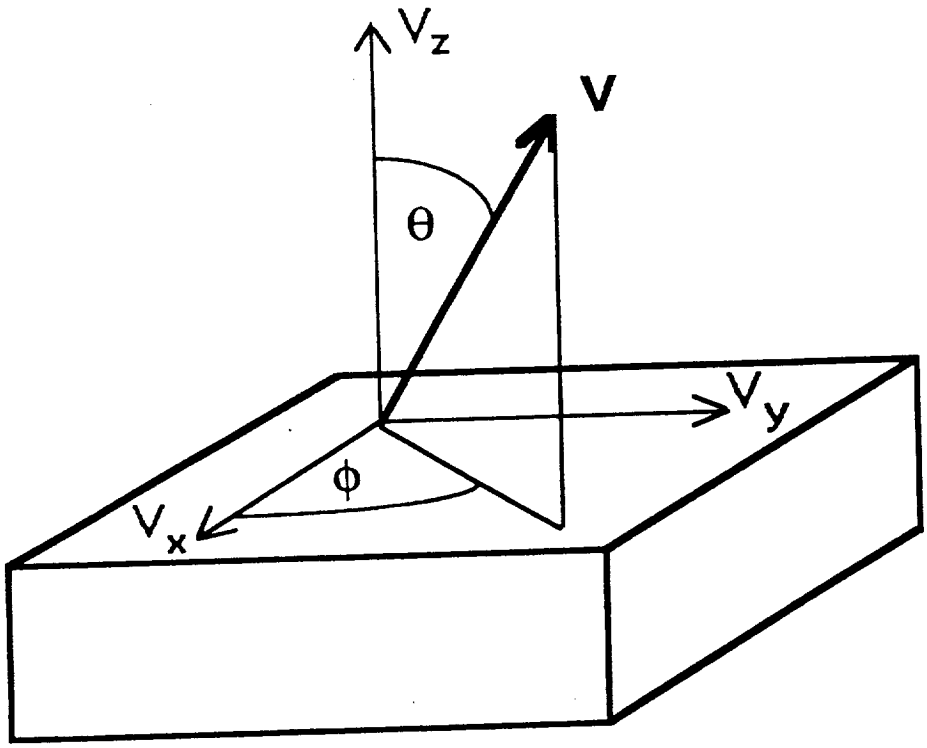


Fig. 13 A secondary electron being emitted from solid bulk material.

F. Determining Velocity Components of Each Secondary Electron

When all the secondaries have been assigned an energy and direction, the only remaining task is to determine the components of velocity for each secondary electron. Recalling equation (2.7), we find the magnitude of the secondary electron's velocity as:

$$V_S = \left(\frac{2 \times E_s \times 1.602189 \times 10^{-19}}{m_e} \right)^{1/2} \quad m/s \tag{2.50}$$

Then the velocity components are given by (Fig. 13):

$$V_x = V \times \sin(\theta) \times \cos(\phi)$$

$$V_y = V \times \sin(\theta) \times \sin(\phi)$$

$$V_z = V \times \cos(\theta) \tag{2.51}$$

III. Concluding Remarks

The procedures outlined in Part II and the FORTRAN code in Appendix C were developed to realistically simulate secondary electron emission in bulk solids caused by incident electrons in a space environment. We have made no attempt to include secondary electron emission for materials in any other physical form, or emission induced by other particles or photons, or high temperatures. The interested researcher is referred to the literature for such cases. Our model will produce realistic results for primary electron energies between 0.0 eV and 1.0 keV with an angle of incidence between 0.0 and $\pi/2$ radians. However, some words of caution are in order.

First, the experimental and simulation data we used to develop our distribution functions and yield curves are generally from coarse data with the first data point at 50 or 100 eV and the highest at 1.0 or 1.2 keV. Experimental data for low energy primary electrons collected by Bruining show fine structure in the secondary electron yield δ, whereas the smooth curve obtained from equation (2.1) is actually an extrapolation back to 0.0 from 50 eV. But since the shape of the fine structure is dependent on the type of material and the fine structure in the actual yield curves produces little variation from equation (2.1), we decided to ignore such features in order to gain breadth of applicability. By running some additional simulations with Rezvani's programs at low E_p (0 to 40 eV), we have been able to describe the behavior of SEE in this region more realistically. The description of section IIC now gives a good picture of the phenomena involved with low energy primaries.

Second, Bruning suggests that as the primary electron energy increases from 0.0 eV to some small value the probability that the primary electron suffers specular reflection increases. But the discussion of this in the literature is sparse, and little quantitative information is available. Fortunately the new runs with Rezvani's programs demonstrate the behavior of reflected primaries (elastically backscattered primary electrons) very nicely. The large yield of reflected primaries for $E_p < 10$ eV, as described in section IID, will have a noticeable effect in the plasma simulations for solar panels.

Third, the secondary electron energy distribution function we developed effectively goes to 0.0 at 30.0 eV with 8-bit floating point numbers. Our distribution is certainly good for simulations where the primary electron energy is less than 1.0 keV. However at higher energies the number of inelastically backscattered primary electrons increases, but our distribution (and Rezvani's model) does not account for the characteristic elastically backscattered primaries at larger primary energies ($E_p > 100$ eV). If these cases are to be accounted for we suggest development of

another distribution that will account for the required higher secondary energies. Then the programmer can choose between our energy distribution or the new one in an IF block as needed.

Fourth, the literature generally subscribes to a cosine distribution for the angular distribution of the secondary electrons. This form was used by early researchers in this field and has remained the traditional distribution. We, on the other hand, have fit the distribution function of eq. (2.22) to the simulation results. There is actually not a great deal of difference between our angular distribution and a cos θ distribution. We believe that our distribution is somewhat more realistic in representing enhanced emission at forward angles, near the normal direction.

The plots on the following pages are from several runs of our simulations at designated energies of the primary electron; E_p is set in the routine SECONDARIES and θ_p is maintained at zero. All the simulations were run with a sum total of less than 35 seconds of CPU time.

All the plots show the behavior for model quartz, with band gap $E_g = 8.0$ eV. The first three figures give the yield δ versus primary energy E_p from 0 to 50 eV. The influence of the finite band gap in reducing the yield of true secondaries for $E_p < 15$ eV is evident in the first plot. The second plot shows the importance of reflected primaries for $E_p < 15$ eV, and the third plot gives the combined results for all electrons coming back from the surface.

The next four figures show the energy distribution of the secondary electrons. At low primary energies ($E_p = 9$ and 14 eV) the influence of the band gap on the energy distribution is readily apparent. At larger primary energies (30 and 50 eV), the only noticeable effect is the backscattered peak at $E_s = E_p$.

The angular distribution of the secondary electrons is shown in the last two figures. The distribution for the polar angle is peaked somewhat toward the normal ($\theta = 0°$, $\cos\theta = 1$), as discussed previously.. The distribution for the azimuthal angle is flat, as expected, with $p(\phi) = p_o = 1/(2\pi) = 0.159$.

As can be seen on the plots, the simulation results follow well the analytic distributions and arguments of Part II. Providing correct results with a minimum of CPU time is the best that can be expected of a numerical simulation of this nature. For this we have strived and, within the limits of our model, this we have obtained.

A. References

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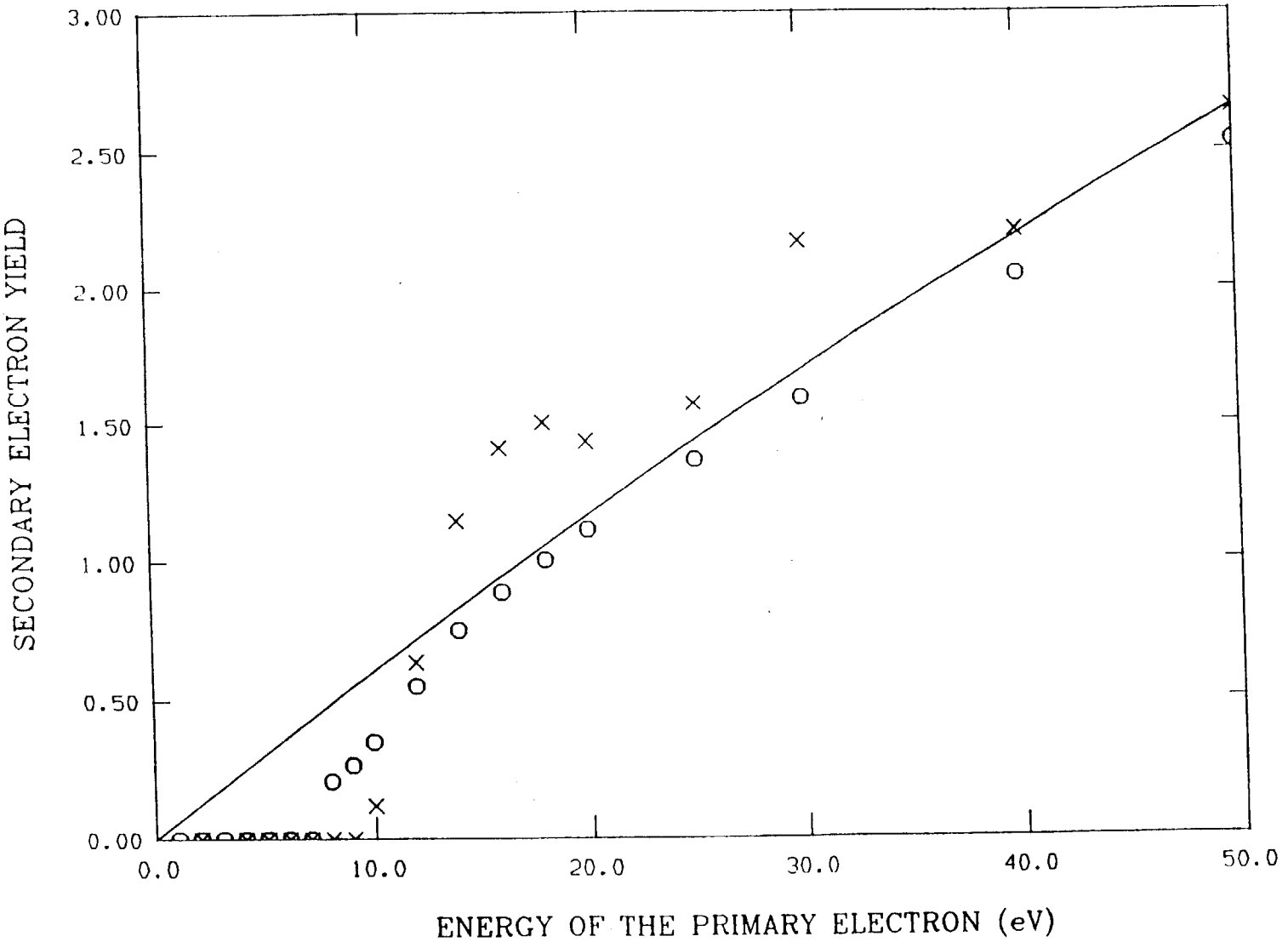

Fig. 14 Yield of secondary electrons *vs.* primary electron energy. The X's are from Rezvani's simulation of the SEE process for quartz. The solid line is from the Haffner formula fitted to these results. The O's show results from our procedures as described in the text, where the yield of secondary electrons at low primary energies is limited by the finite band gap of the insulator.

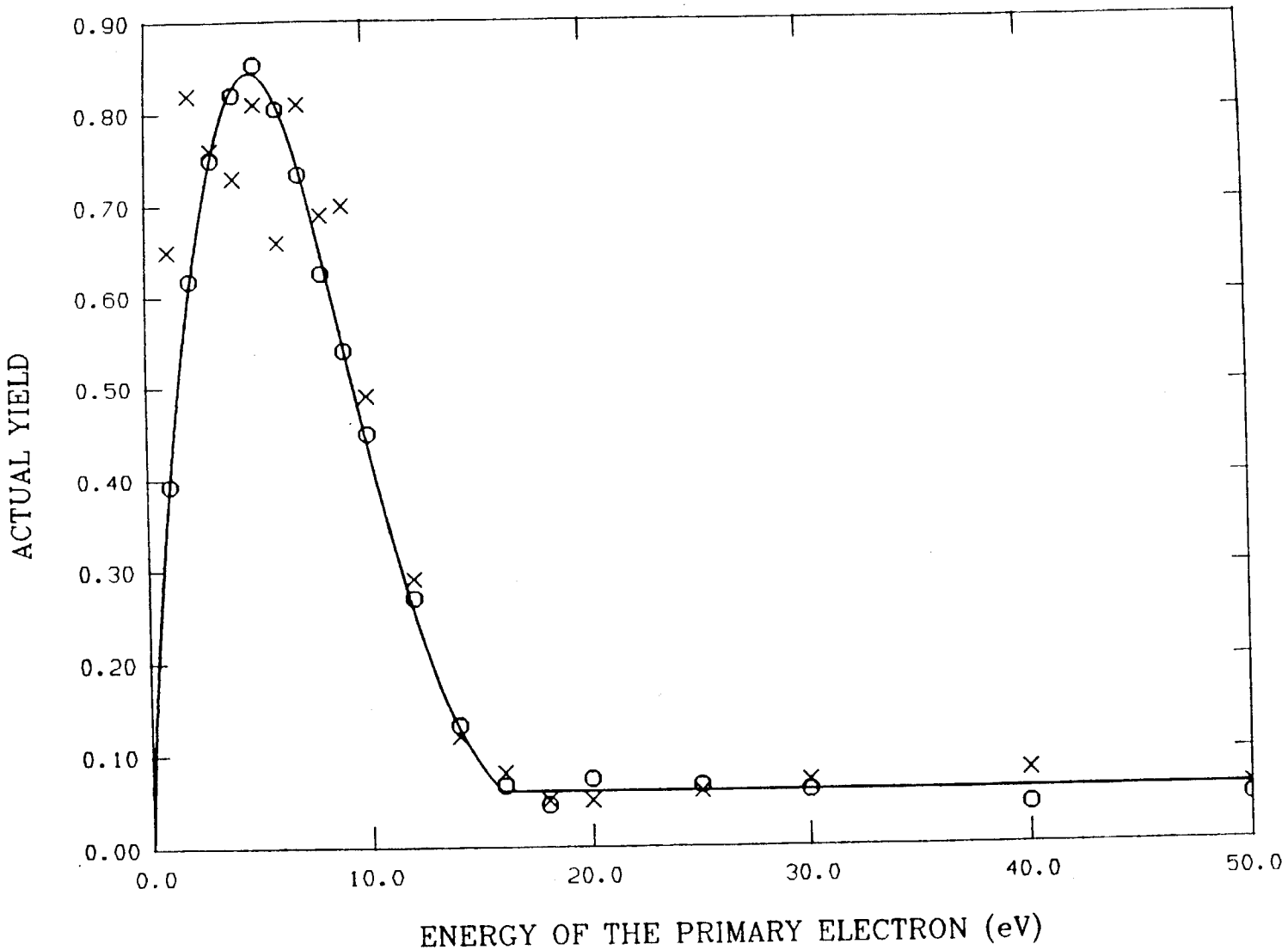

Fig. 15 Yield of reflected primary electrons *vs.* primary electron energy for quartz. The symbols and procedures are described in Fig. 14. Here the solid line is from the empirical formula for reflected electrons as given in the text.

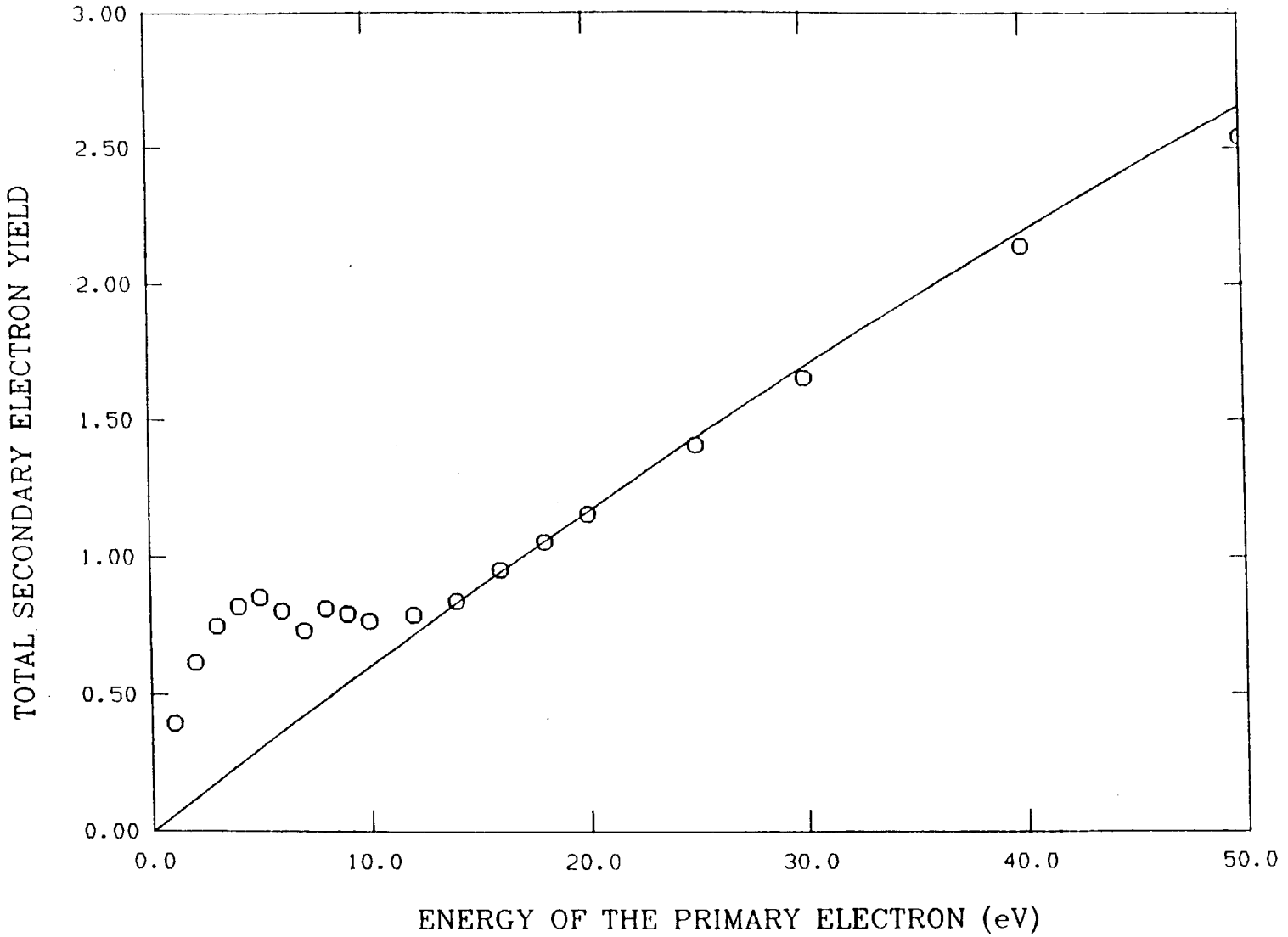

Fig. 16 Total yield of secondary electrons for quartz. These are the combined results for secondary electron emission from Fig. 14 and for reflected primary electrons from Fig. 15. The O's show the results from our procedures, and the solid line is from the Haffner formula.

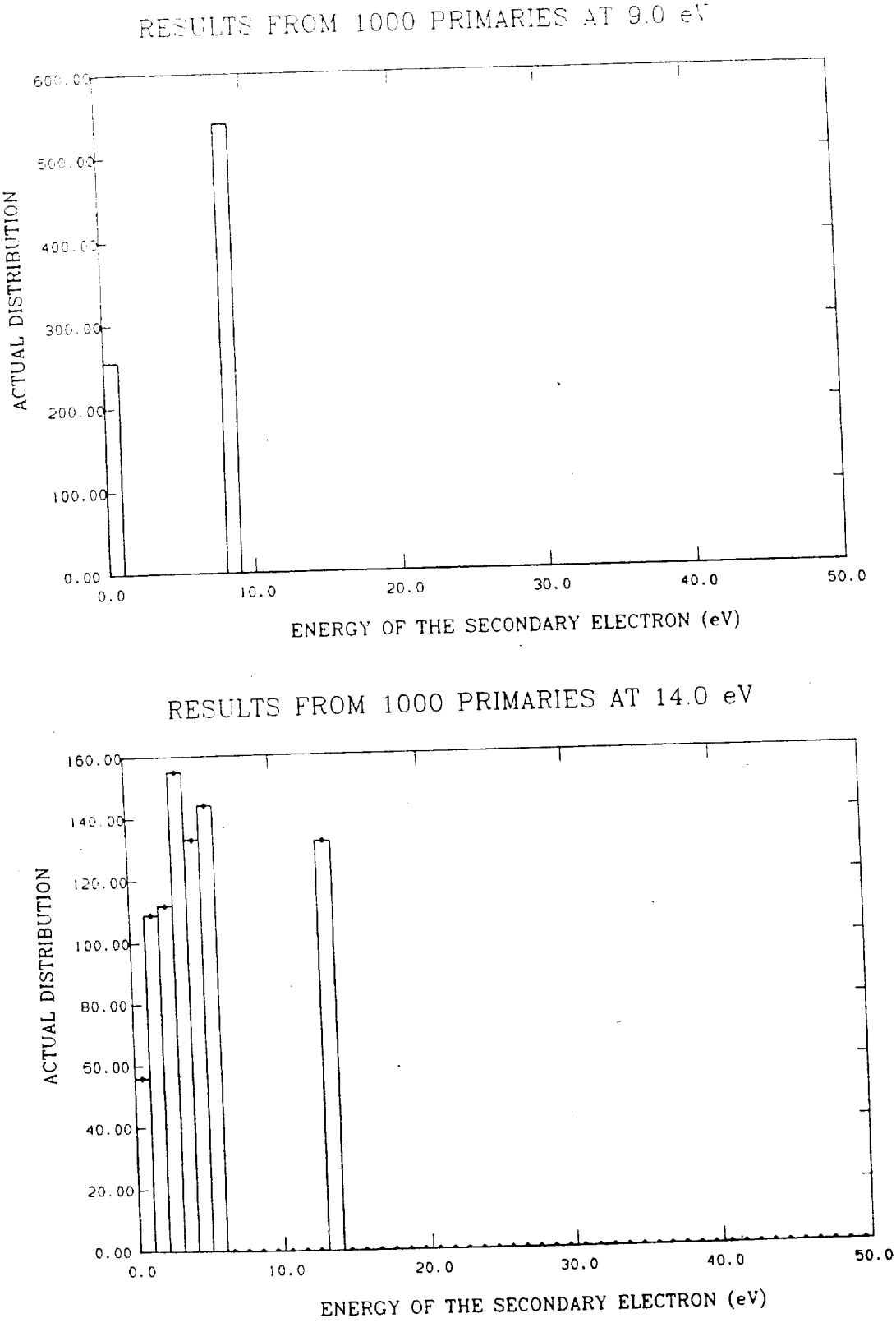

Fig. 17 Energy distribution of secondary electrons for primary energies of 9.0 eV and 14.0 eV.

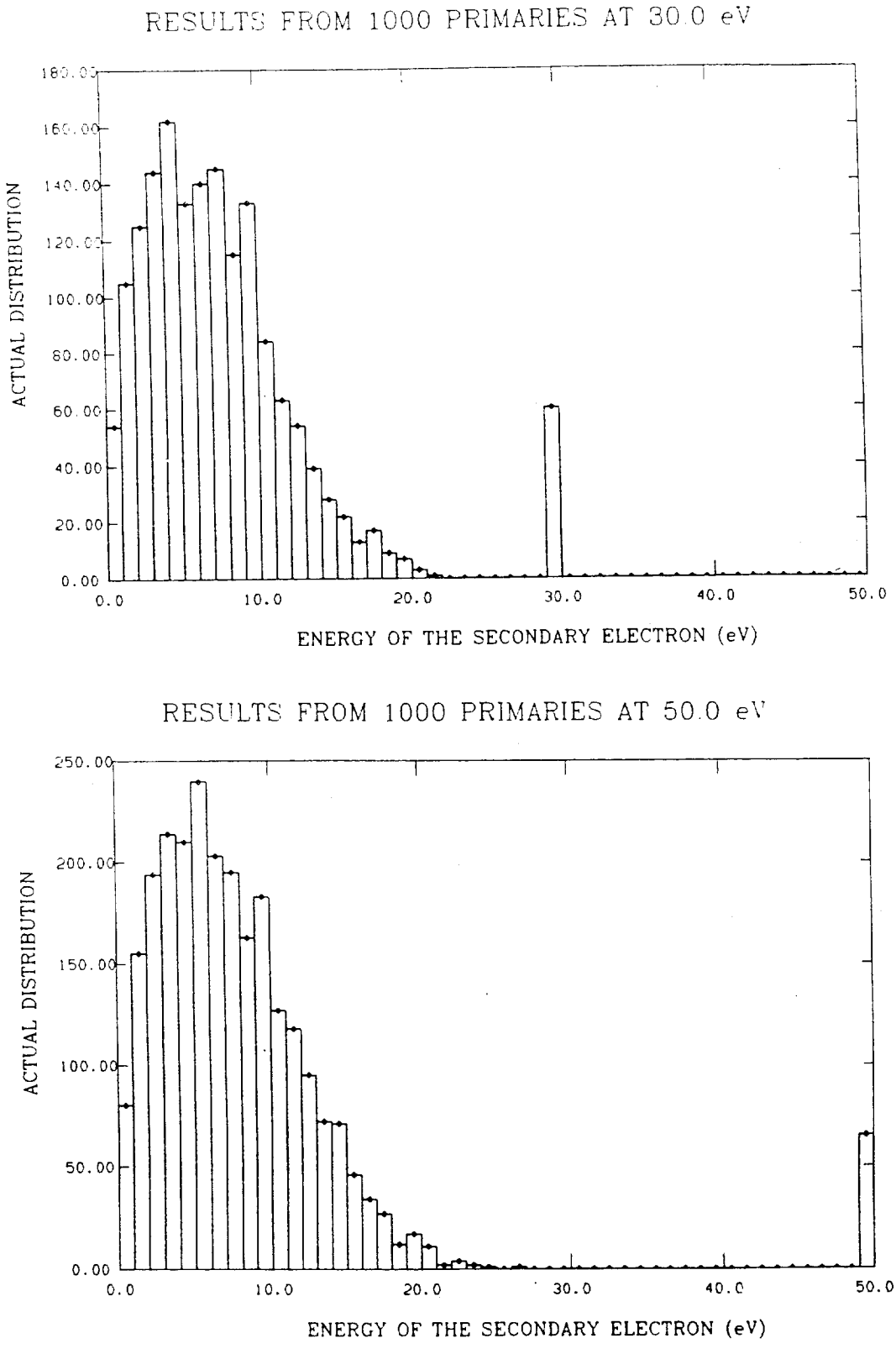

Fig. 18 Energy distribution of secondary electrons for primary energies of 30.0 eV and 50.0 eV.

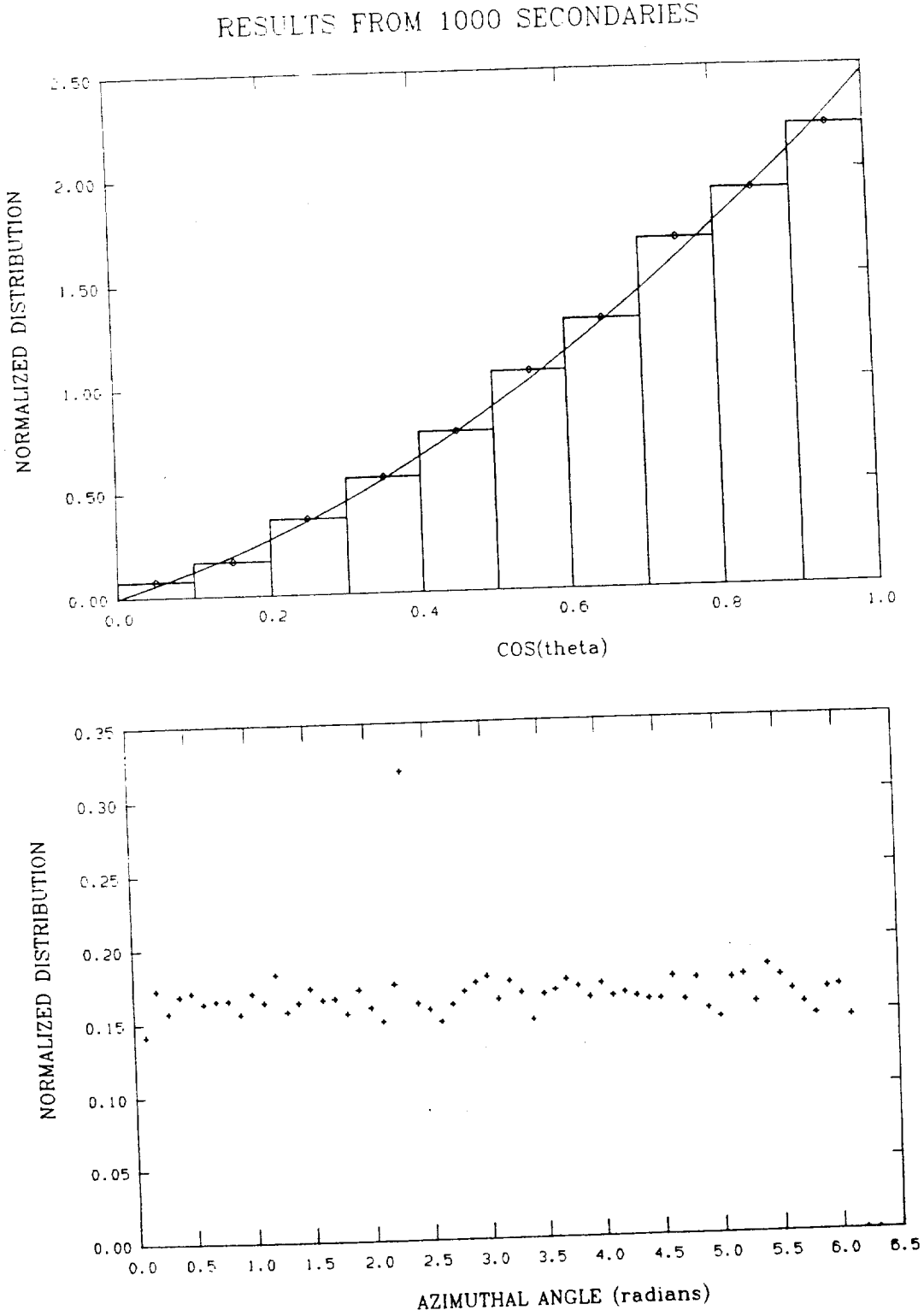

Fig. 19 Angular distribution of secondary electrons. The upper distribution for the polar angle θ is slightly more peaked in the forward direction than a simple $\cos\theta$ distribution. The lower distribution for the azimuthal angle ϕ is uniform as expected.

C. FORTRAN Programs

```
c=====================================================================
c                        subroutine  SECDATA
c
c This subroutine is used to input  the data files for secondary electron
c emission.  It is used only once at  the beginning of a simulation.
c
c  sec_energy_file2              the data of secondary energy vs. probability
c  sec_theta_file                the data of secondary angle vs. probability
c  sec_energy_file               the data of probability vs. secondary energy
c=====================================================================
c
        subroutine secdata
c
        common /energy/ AREAeng(3001),VALUEeng(3001)
        common /angle/ AREAthe(501),VALUEthe(501)
        common /energy2/ AREAeng2(1001),VALUEeng2(1001)
c
        open(unit=92,file='sec_energy_file2.dat',status='old')
        open(unit=91,file='sec_theta_file.dat',status='old')
        open(unit=90,file='sec_energy_file.dat',status='old')
        do i=1,3001
                read(90,*)VALUEeng(i),AREAeng(i)
                if(i.lt.502)then read(91,*)AREAthe(i),VALUEthe(i)
                        end if
                if(i.lt.1002)then read(92,*)AREAeng2(i),VALUEeng2(i)
                        end if
                end do
        close(unit=90)
        close(unit=91)
        close(unit=92)
c
        return
        end
c=========================end of secdata=============================

c=====================================================================
c                        subroutine SECONDARIES
c
c Secondary Electron Emission
c
c Given on input the primary electron's velocity components  [Vx], [Vy], and [Vz], and
c  an integer value  [MAT]  to indicate the type of material involved, and an integer
c  value  [BOUND] to indicate the boundary surface, this routine will calculate the
c  primary electron's kinetic energy  [Ep]  and its angle of incidence  [THETAP].  This
c  routine will also determine the probability of the primary electron elastically
c  reflecting with a call to  "YIELDMAX".
c
```

```
c Afterwards, the secondary electron production calculations will begin with a call to
c "YIELDMAX," which will calculate a secondary electron [YIELD] based on the
c  Haffner  formula. This real number is added to a random number less than one and
c  the sum is truncated to an integer.  This integer is considered to be the total
c  possible secondary yield  [Npos].
c
c This routine will then call a second routine called "SECENERGY" to assign an
c energy  [Es]  to each secondary electron. To conserve the energy delivered to the
c material by the primary electron,  [Ep] + Ki  will be considered the maximum amount
c of energy available to all the possible secondaries. Each (Jth) secondary will
c receive an energy from a Monte Carlo method until there is no longer enough
c energy to allow the (Jth+1) secondary to overcome the material's surface barrier,
c or until J = [Npos].
c
c Then a third routine called  "SECANGLES"  will be called to assign the angles
c  [THETAS]  and  [PHES]  to each secondary that had enough energy to overcome
c the surface barrier.  [THETAS]  will be choosen with a Monte Carlo method first,
c  then  [PHES] will be choosen at random.
c
c With the angles and energies of each secondary now assigned, this routine will call
c its final subroutine  "SECVELOCITIES"  to assign velocity components  [Ux], [Uy],
c and [Uz]  that are consistent with each secondary's assigned angles and energy.
c
c With all calculations now complete this routine will return the values  [Nact],  which
c is the actual secondary electron yield, and the velocity components  [Ux], [Uy], and
c [Uz],  which are arrays of dimension  [Nact].
c
c If  [Nact] = 0 then no secondaries were produced, but the primary stuck to the
c  material.  If  [Nact] = -1 then no secondaries were produced, and the primary was
c reflected from the material. A postive value for  [Nact]  indicates the actual number
c of secondaries produced, and that the primary stuck to the material.
c=================================================================
c
      subroutine secondaries(I,Vx,Vy,Vz,mat,bound,Uxx,Uyy,Uzz,Nact)
c
      real Vx,Vy,Vz,thetap,Ep,Ki      ! Values of the primary electron
      integer bound,mat               ! Indicates the type of material
      integer I                       ! The passed random number argument
c
      real Uxx(30),Uyy(30),Uzz(30)    ! Secondary velocity
      real thetas(30),phes(30)        ! Secondary angular direction
      real Es(30)                     ! Energy of each secondary
      real yield                      ! Value from the Haffner formula
      integer Nact,Npos               ! Actual and possible yields
c
      logical reflect
c
```

```
c   assign values to  a, b, c, and Eg   for Haffner formula
c
        if(mat.eq.1)then                ! The material is QUARTZ
                a  = 1.02
                b  = 5.47               ! Eg is the band gap energy
                c  = 14.02
                Eg = 8.0                ! Wf is the work function
                Ki = 1.0
                Wf = 0.0
        else if(mat.eq.2)then           ! The material is
                a  = 2.0
                b  = 15.0               ! Holmes-insulator
                c  = 4.72
                Eg = 4.0                ! Ki is the electron affinity
                Ki = 1.0
                Wf = 0.0
        else if(mat.eq.3)then           ! The material is Holmes-metal
                a  = 0.1
                b  = 10.0               ! a, b, and c are parameters
                c  = 2.12
                Eg = 0.0                ! for the Haffner formula
                Ki = 0.0
                Wf = 5.0
        else if(mat.eq.4)then           ! The material is ALUMINIUM
                a  = 0.5
                b  = 8.3
                c  = 1.23
                Eg = 0.0
                Ki = 0.0                ! This value of Wf is from
                Wf= 4.25                ! Rezvani thesis, Vol 1, page 206
        end if
c
c  calculate the energy and angle of incidence of the primary
c
        Vsqrd = ((Vx ** 2) + (Vy ** 2) + (Vz ** 2))
        energ = 0.5 * 9.109534E-31 * Vsqrd          ! Ep in JOULES
        Ep = energ/(1.6021892E-19)                  ! Ep in eV
c
        if ((bound .eq. 1) .or. (bound .eq. 3) .or.  (bound .eq. 5)) then
                thetap = atan(sqrt((Vx ** 2) + (Vy ** 2))/-Vz)
        else if (bound .eq. 2) then
                thetap=atan(sqrt(Vx**2+Vz**2)/Vy)
         else if (bound .eq. 4) then
                thetap=atan(sqrt(Vx**2+vz**2)/-Vy)
        end if
c
c       write(16,*)'--------------------------------'
c       write(16,*)'ep=',ep,'  thetap=',thetap
c
```

```
c calculate the possibility of reflection
c
      if (mat .EQ. 1 .OR. mat .EQ. 2)then
            call elasref(I,Ep,reflect)                ! Reflection
            if(reflect)then                           ! The reflection is elastic,
                  Nact = 1                            ! but not specular
                  Es(1) = Ep
                  call secangles(I,Nact,thetas,phes)
                  call secvelocities(bound,Nact,Es,thetas,phes,Uxx,Uyy,Uzz)
                  Nact = -1
                  return
            end if
      end if
c
c  calculate the total possibile yield
c
      y = ran(I)
      call yieldmax(a,b,c,Ep,thetap,yield)      ! This is the integer value of
      Npos = int(yield + y)                     ! secondaries that may be produced.
c
c  assign an energy to each secondary and find [Nact]
c
      call secenergy(I,Ep,Eg,Ki,Wf,Npos,Es,Nact)
c
c The remaining energy may be considered to have been absorbed by the crystal
c lattice.  Thus Ep is now  zero and the primary is "STUCK."
c
      if(nACT.eq.0) then                        ! Even though there existed the possibility of
            return                              ! producing secondaries, because of  energy
      end if                                    ! considerations none were produced.
c
c assign the directional angles to each secondary
      call secangles(I,Nact,thetas,phes)
c calculate the components of the velocities for the secondaries
      call secvelocities(bound,Nact,Es,thetas,phes,Uxx,Uyy,Uzz)
c all calculations are complete for that primary electron
c
c     write(16,*)'npos=',npos,' nact=',nact
c     do i=1,nact
c        write(16,*)'i=',i,' es=',es(i),' thetas',thetas(i)
c     end do
      return
      end
c=========================end of secondaries==========================

c=======================================================================
c                       subroutine SECANGLES
c
c This routine will assign values to the spherical-polar angular
c  coordinates theta and phe for each secondary electron.
```

```
c  The azimuthal angle, theta, will be generated with a Monte
c  Carlo method using the distribution function:
c
c       Y = A COS(theta) + B COS^2(theta) + C COS^3(theta)
c
c where the parameters  A,B, and C  are determined by a best fit  to G. A. Rezvani's
c  secondary electron angular distribution data for runs at  50 eV  and  400 eV.
c  The polar angle, phe, will be chosen at random since the determination of
c  phe = 0.0  is arbitrary to the plasma simulation.
c=====================================================================
c
        subroutine secangles(I,Nact,thetas,phes)
c
        integer Nact
        real thetas(30),phes(30),rtheta
c
c  find the angles
c
        do i=1,Nact
                rtheta = ran(I)
                call find_theta(rtheta,thetas(i))
                phes(i) = ran(I) * (2 * 3.141593)
        end do
c
        return
        end
c========================== end of secangles ===========================

c=====================================================================
c                           subroutine SECVELOCITIES
c
c  This routine will assign values to the velocity components
c  [Ux], [Uy], and [Uz]  for each secondary electron,  [Ys].
c
c  For each secondary electron the magnitude of the total velocity [V] is calculated
c  from a knowledge of its total energy  [Es].  Then each component is calculated
c  according to the following equations:
c             Uz = V * cos(theta)
c             Uy = V * sin(theta) * sin(phe)
c             Ux = V * sin(theta) * cos(phe)
c=====================================================================
c
        subroutine secvelocities(bound,Nact,Es,thetas,phes,Uxx,Uyy,Uzz)
c
        integer Nact,bound
        real Es(30),Uxx(30),Uyy(30),Uzz(30),thetas(30),phes(30)
        real m,V
c
        m = 9.109534E-31
        c = 1.602189E-19
```

```
        do i=1,Nact
                        V = sqrt((2 * Es(i) * c)/m)
                        Uxo = V * sin(thetas(i)) * cos(phes(i))
                        Uyo = V * sin(thetas(i)) * sin(phes(i))
                        Uzo = V * cos(thetas(i))
c
                if ((bound.eq.1).or.(bound.eq.3).or.(bound.eq.5)) then
                        Uxx(i)=Uxo
                        Uyy(i)=Uyo
                        Uzz(i)=Uzo
                else if (bound.eq.2) then
                        Uxx(i)=Uxo
                        Uyy(i)=-Uzo
                        Uzz(i)=Uyo
                else if (bound.eq.4) then
                        Uxx(i)=Uyo
                        Uyy(i)=Uzo
                        Uzz(i)=Uxo
                end if
        end do
        return
        end
c========================= end of secvelocities ======================

c=====================================================================
c                       subroutine SECENERGY
c
c  This routine assigns an energy [Es] to the secondary electrons.  The information
c   that comes from the calling routine is the total avaliable energy  [Eavail],  the
c   threshold energy from the material's band gap  [Eg]  and electron affinity  [Ki],  and
c   the total possible yield from the (modified) Haffner formula.  This routine will loop
c  until all the electrons given by the Haffner formula have been assigned an energy,
c  or until  the energy equation cannot be satisfied:
c
c          Eavail = > Ki + Eg + Es(I) + sum[Es(I-1) + Eg + Ki]   (1)
c
c  Since each secondary must overcome the surface barrier, it will lose an amount of
c  energy equal to  Eg + Ki  before it is outside the material. The sum of the energies
c  assigned  to each secondary plus the sum of the energy  lost as each secondary
c  crosses the surface barrier must not be greater than the energy delivered to the
c  material by the primary electron.  That way energy is conserved.  After going
c  through this loop as many times as possible any "left over" energy will  be
c  considered to be absorbed by the crystal lattice, again conserving energy.
c
c  The distribution function that will be used to assign secondary energies is from
c   the best fit to G. A. Rezvani's data on secondary energy:
c
c          f(Es) = A(Es^0.5)exp[-(Es/Eo)^2]       (2)
c
```

```
c A random number will be chosen and will be associated with the integral of the
c distribution function from zero to some  Es,  which is normalized for energies
c between 0 and some  [Emax]. Once this area is known, a call to "FIND_ENERGY"
c will give the value of Es(l). If Es(l) doesn't  satisfy equation (1), Ep is considered
c to be exhausted.
c=====================================================================
c
      subroutine secenergy(l,Eavail,Eg,Ki,Wf,Npos,Es,Nact)
c
      real Eavail, Eg, Ki, Wf, Eo, Es(30)
      real dlEmax, Emax, rarea
      integer Npos, Nact
c
c calculate Es and the actual_yield
c
      Nact = 0                          ! The magnitude of the surface barrier.  For
      Eo = Eg + Ki + Wf                 ! insulators, Eo is the sum  Eg + Ki.  For metals,
                                        ! Eo is just the work  function.
c
      dlEmax = Eavail + Ki + Wf         ! The maximum energy deliverable to
                                        !  interactions with the secondaries.
      if (npos .gt. 30) npos=30
      do i=1,npos
            Emax = dlEmax - Eo          ! The total possible energy the secondary
                                        ! under consideration can have.
            if(Emax.lt.0)return         ! There is not enough energy to get
                                        ! another secondary past the surface barrier.
            rarea = ran(l)
            call find_energy(rarea, Emax, Es(i))
c
            dlEmax = Emax - Es(l)       ! The total deliverable energy less the amount
                                        ! delivered to the secondary being considered.
            Nact = i                    ! An actual secondary has been observed.
      end do
      return
      end
c=========================end of secenergy============================

c=====================================================================
c                       subroutine  FIND_ENERGY
c
c This routine selects an energy for the secondary in accordance with
c  the distribution function described in the text.
c=====================================================================
c
      subroutine find_energy(proba,Emax,eng).
c
      real proba,Emax,eng
      common /energy/AREAeng(3001),VALUEeng(3001)
      common /energy2/ AREAeng2(1001),VALUEeng2(1001)
```

```
      proba1=proba
      if (Emax .lt. 30.0) then
            j=int(Emax*100)+1
            Pmax=AREAeng(j)+(Emax-VALUEeng(j))*(AREAeng(j+1)
     &           -AREAeng(j))/(VALUEeng(j+1)-VALUEeng(j))
            proba1=proba1*Pmax
      end if
c
      index=int(proba1*1000)+1
      eng=VALUEeng2(index)+(proba1-AREAeng2(index))*(VALUEeng2(index+1)
     &     -VALUEeng2(index))/(AREAeng2(index+1)-AREAeng2(index))
c
      return
      end
c=========================end of find_energy============================

c=====================================================================
c                     subroutine  FIND_THETA
c
c This routine selects a value of theta for the secondary electron.
c=====================================================================
c
      subroutine find_theta(proba,angler)
      common /angle/ AREAthe(501),VALUEthe(501)
c
      index=int(500.0*proba)+1
      angler=VALUEthe(index)+(proba-AREAthe(index))*(VALUEthe(index+1)
     &     -VALUEthe(index))/(AREAthe(index+1)-AREAthe(index))
      return
      end
c=========================end of find_theta=============================

c=====================================================================
c                     subroutine YIELDMAX
c
c This program will make use of the angular modified Haffner formula:
c
c       Yield(E) = C[EXP(-aE) - EXP(-bE)]*EXP(1 - COS(THETA))
c
c to calculate the secondary electron [YIELD] as a function of the primary electron
c [ENERGY] and angle of incidence [THETA].
c=====================================================================
c
      subroutine yieldmax(a,b,c,energy,theta,yield)
      real yield,energy,c,a,b,theta
c
      energy = energy/1000                    ! convert Ep from eV's to keV's
      aterm = exp(1-cos(theta))
      yield = c * ((exp(-a * energy))-(exp(-b *energy))) * aterm
      energy = energy * 1000                  ! convert Ep back to eV's
```

```
      return
      end
c=========================end of yieldmax=============================

c=========================================================================
c                     subroutine ELASREF
c
c This routine will take an empirical formula fit to G. A. Rezvani's simulation data for
c elastic reflection of the primary electron at a broad number of energies between
c 1.0 and 50.0 eV. Since the result of the equation is always a fraction and since the
c primary must reflect or not reflect on an all or nothing basis, we will add a random
c fraction to the result of the formula, take the integer part and truncate it to an
c integer. If the result of this proceedure is one, we consider the primary electron to
c have suffered elastic reflection. If the result is zero, there is no reflection.
c=========================================================================
c
      subroutine elasref(I,Ep,reflect)
c
      real Ep
      integer I,i,ichance
c
      logical reflect
      reflect = .false.
c
      a = 0.40                          ! These are from a fit to Rezvani's data
      B = 0.70                          ! for Ep equal to or less than 17 eV.
      c = 8.1
      d = 2.0
c
      if(Ep.lt.16.88)then
            y = a * (eP**b) * exp(-(eP/c)**d)
      else
            y = 0.06                    ! At higher energies, Rezvani's data flatten out.
      end if
c
      ichance = int(y + ran(I))         ! The chance to reflect
      if(ichance.gt.0)reflect = .true.
c
      return
      end
c=========================end of elasref=============================
```

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16. Abstract

Previous Monte Carlo simulations provide a data base for properties of secondary electron emission (SEE) from insulators and metals. Incident primary electrons are considered at energies up to 1200 eV. The behavior of secondary electrons is characterized by (1) yield vs. primary energy E_p, (2) distribution vs. secondary energy E_s, and (3) distribution vs. angle of emission θ. Special attention is paid to the low energy range E_p up to 50 eV, where the number and energy of secondary electrons is limited by the finite band gap of the insulator. For primary energies above 50 eV the SEE yield curve can be conveniently parameterized by a Haffner formula. The energy distribution of secondary electrons is described by an empirical formula with average energy about 8.0 eV. The angular distribution of secondaries is slightly more peaked in the forward direction than the customary cos θ distribution. Empirical formulas and parameters are given for all yield and distribution curves. Procedures and algorithmms are described for using these results to find the SEE yield, and then to choose the energy and angle of emergence of each secondary electron. These procedures can readily be incorporated into numerical simulations of plasma-solid surface interactions in low earth orbit.

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